

**Electronic structure and luminescence properties of unique  
complexes: cyclometalating iridium(III) chelated by o-carboranyl-  
pyridine ligand**

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**Table S1.** Selected bond lengths [ $\text{\AA}$ ], bond angles [deg] at  $S_0$  optimized geometry for complex **1**.

	B3LYP	PBE0	M052X	M062X	BMK	CAM-B3LYP	Exp. <sup>a</sup>
Ir-C(1)	2.236	2.192	2.191	2.209	2.193	2.212	2.175
Ir-C(8)	2.057	2.038	2.038	2.031	2.071	2.049	2.055
Ir-C(19)	2.015	1.999	1.992	1.984	2.021	2.008	2.030
Ir-N(1)	2.290	2.235	2.262	2.297	2.242	2.259	2.227
Ir-N(2)	2.114	2.084	2.106	2.112	2.136	2.104	2.098
Ir-N(3)	2.075	2.048	2.063	2.063	2.107	2.067	2.039
C(1)-C(2)	1.680	1.660	1.647	1.655	1.793	1.660	1.703
C(2)-C(3)	1.499	1.492	1.494	1.499	1.510	1.496	1.512
C(1)-Ir-N(1)	77.33	78.18	77.98	77.32	79.47	77.84	78.60
C(1)-Ir-C(19)	96.36	95.82	95.72	95.95	94.81	96.13	95.70
C(8)-Ir-N(1)	93.04	92.74	92.77	93.10	93.03	93.06	92.30
C(8)-Ir-C(19)	93.43	93.39	93.61	93.73	92.96	93.10	93.50
C(1)-Ir-N(2)	99.02	99.06	99.55	99.32	98.66	99.32	99.00
C(8)-Ir-N(2)	78.92	79.21	79.24	79.31	78.86	79.01	80.40
C(19)-Ir-N(2)	93.26	93.02	93.29	93.40	92.09	92.94	92.10
N(1)-Ir-N(2)	92.73	92.65	92.61	92.63	94.79	92.96	93.60
C(1)-Ir-N(3)	91.91	91.89	91.52	91.28	93.05	91.90	93.20
C(8)-Ir-N(3)	91.20	90.83	90.64	91.03	90.42	90.80	88.60
C(19)-Ir-N(3)	80.12	80.37	80.53	80.67	80.11	80.17	80.20
N(1)-Ir-N(3)	94.91	94.95	94.62	94.37	94.01	94.93	95.10
N(2)-Ir-N(3)	167.83	167.76	167.84	168.37	166.46	167.44	166.20

<sup>a</sup> Experimental data is obtained from ref. 29**Table S2.** Calculated maximum emission wavelengths ( $\lambda_{\text{max}}$ , nm) for complex **1** with different functionals.

nm	B3LYP	PBE0	M062X	M052X	BMK	CAM-B3LYP	Exp. <sup>a</sup>
$\lambda_{\text{em}}$	573	571	482	508	465	559	517

<sup>a</sup> Experimental data is obtained from ref. 29

**Table S3.** The analysis of the molecular orbital compositions in the lowest-lying triplet state for all complexes at the TDDFT/M052X level.

Orbitals	transitions (%)	Energy (eV)	MO compositions				Composition contribution > 11%	
			(C^N)1	(C^N)2	Ir	CBpy		
<b>1</b>	H-1	H-1→L (50%)	-7.25	23	68	5	4	(C^N)1+C^N)2
	H	H→L (37%)	-6.46	40	24	27	8	(C^N)1+(C^N)2+Ir
	L		-1.03	1	92	4	3	(C^N)2
<b>2</b>	H-1	H-1→L (29%)	-7.28	30	58	10	2	(C^N)1+(C^N)2
	H	H→L (42%)	-6.25	40	22	28	11	(C^N)1+(C^N)2+Ir
	L		-1.2	1	94	4	1	(C^N)2
<b>3</b>	H-1	H-1→L (11%)	-7.1	22	71	6	2	(C^N)1+(C^N)2
	H	H→L (58%)	-6.28	66	12	17	5	(C^N)1+(C^N)2+Ir
	L		-1.15	90	7	1	2	(C^N)1
<b>3a</b>	H	H→L (41%)	-6.27	55	15	22	7	(C^N)1+(C^N)2+Ir
	L	H→L+1(13%)	-1.01	60	36	2	2	(C^N)1+(C^N)2
	L+1		-0.86	35	60	3	3	(C^N)1+(C^N)2
<b>4</b>	H-1	H-1→L (13%)	-0.8	35	53	11	1	(C^N)1+(C^N)2
	H	H→L (60%)	-6.18	75	7	13	4	(C^N)1+Ir
	L		-1.04	96	2	1	1	(C^N)1
<b>4a</b>	H	H→L (86%)	-6.13	85	4	9	2	(C^N)1
	L		-1.06	89	2	3	5	(C^N)1
<b>5</b>	H-1	H-1→L (23%)	-6.97	41	52	5	1	(C^N)1+(C^N)2
	H	H→L (46%)	-6.32	62	13	20	5	(C^N)1+(C^N)2+Ir
	L		-1.31	96	1	1	2	(C^N)1

	H-1	H-1→L (35%)	-6.78	43	39	13	5	(C <sup>^</sup> N) <sub>1</sub> +(C <sup>^</sup> N) <sub>2</sub> +Ir
<b>5a</b>	H	H→L (61%)	-6.61	20	60	17	2	(C <sup>^</sup> N) <sub>1</sub> +(C <sup>^</sup> N) <sub>2</sub> +Ir
	L		-1.66	0	95	3	1	(C <sup>^</sup> N) <sub>2</sub>

**Table S4.** Transition dipole moments  $\mu(S_n)$  (Debye) for  $S_0$ - $S_n$  transitions, singlet-triplet splitting energies  $\Delta E(S_n-T_1)$  (eV) and the SOC matrix elements  $\langle S_n | H_{\text{soc}} | T_1 \rangle$  of all complexes.

$S_n$	<b>1</b>			<b>2</b>		
	$\mu(S_n)$	$\Delta E(S_n-T_1)$	$\langle S_n   H_{\text{soc}}   T_1 \rangle$	$\mu(S_n)$	$\Delta E(S_n-T_1)$	$\langle S_n   H_{\text{soc}}   T_1 \rangle$
$S_1$	1.09	0.34	22.13	2.61	0.38	10.26
$S_2$	0.94	0.80	20.27	2.68	0.45	368.19
$S_3$	0.47	0.88	50.04	3.08	0.85	408.52
$S_4$	0.92	1.15	461.15	3.26	1.03	499.59
$S_5$	0.36	1.20	90.89	3.42	1.20	72.74
$S_6$	0.67	1.34	417.83	3.44	1.21	174.01
$S_7$	0.67	1.38	54.11	1.64	1.21	104.056
$S_8$	0.15	1.48	70.95	1.56	1.30	131.915
$S_9$	0.08	1.59	332.73	0.67	1.42	24.070
$S_{10}$	1.06	1.63	116.60	0.45	1.45	45.150
$S_n$	<b>3</b>			<b>3a</b>		
	$\mu(S_n)$	$\Delta E(S_n-T_1)$	$\langle S_n   H_{\text{soc}}   T_1 \rangle$	$\mu(S_n)$	$\Delta E(S_n-T_1)$	$\langle S_n   H_{\text{soc}}   T_1 \rangle$
$S_1$	0.87	0.65	104.90	1.65	0.29	21.65
$S_2$	0.99	0.80	48.03	0.47	0.40	445.80
$S_3$	0.15	1.16	25.76	0.17	0.81	430.89
$S_4$	0.77	1.41	48.98	0.46	0.86	1037.63
$S_5$	0.77	1.47	177.55	0.58	0.99	6.23
$S_6$	1.09	1.54	91.02	3.07	1.26	195.61
$S_7$	1.59	1.62	181.91	1.40	1.29	3.36
$S_8$	0.56	1.66	16.69	0.35	1.36	21.15
$S_9$	0.39	1.71	831.67	0.65	1.40	24.04
$S_{10}$	0.21	1.74	42.79	1.29	1.42	43.67
$S_n$	<b>4</b>			<b>4a</b>		
	$\mu(S_n)$	$\Delta E(S_n-T_1)$	$\langle S_n   H_{\text{soc}}   T_1 \rangle$	$\mu(S_n)$	$\Delta E(S_n-T_1)$	$\langle S_n   H_{\text{soc}}   T_1 \rangle$
$S_1$	0.90	0.77	63.78	0.73	0.91	58.30
$S_2$	0.54	0.83	12.93	1.67	0.94	23.02
$S_3$	0.19	1.25	6.37	0.40	1.32	40.00
$S_4$	0.23	1.41	28.97	1.08	1.51	14.91
$S_5$	1.57	1.49	87.04	1.90	1.59	101.66
$S_6$	0.98	1.52	64.55	0.32	1.69	71.31
$S_7$	0.63	1.60	19.99	0.30	1.81	71.65
$S_8$	1.19	1.82	129.77	0.97	1.86	162.09
$S_9$	0.11	1.86	12.85	1.40	1.87	41.63
$S_{10}$	0.66	1.86	84.75	0.66	1.91	62.97
$S_n$	<b>5</b>			<b>5a</b>		
	$\mu(S_n)$	$\Delta E(S_n-T_1)$	$\langle S_n   H_{\text{soc}}   T_1 \rangle$	$\mu(S_n)$	$\Delta E(S_n-T_1)$	$\langle S_n   H_{\text{soc}}   T_1 \rangle$
$S_1$	0.68	0.62	106.48	1.37	0.79	191.06
$S_2$	0.22	0.97	22.21	1.40	1.17	106.17
$S_3$	1.12	1.30	19.29	1.38	1.26	16.16

S <sub>4</sub>	0.54	1.33	23.41	0.77	1.43	287.92
S <sub>5</sub>	0.33	1.41	131.99	0.55	1.59	50.58
S <sub>6</sub>	0.75	1.50	144.86	1.59	1.74	183.14
S <sub>7</sub>	1.84	1.67	221.54	0.24	1.76	38.30
S <sub>8</sub>	0.91	1.69	73.90	0.48	1.85	173.18
S <sub>9</sub>	1.35	1.78	155.05	1.25	1.93	256.24
S <sub>10</sub>	0.82	1.80	202.02	1.27	1.99	34.11

**Table S5.** Vibrational frequencies ( $\omega_i/\text{cm}^{-1}$ ) at the respective optimized S<sub>0</sub> states, Shift vector K<sub>i</sub> (a.u.) and Huang-Rhys factor S<sub>i</sub> of complex **1**

	$\omega_i/\text{cm}^{-1}$	K <sub>i</sub> (a.u.)	S <sub>i</sub>
1	31.9653	-1.63E+02	1.94
2	39.5145	1.14E+01	0.01
3	43.2616	8.16E+00	0.01
4	46.0543	3.32E+01	0.12
5	48.6892	2.27E+01	0.06
6	70.6156	-2.33E+01	0.09
7	77.051	-2.99E+01	0.16
8	87.3185	9.41E+00	0.02
9	96.2327	-1.44E+01	0.05
10	117.2739	-1.45E+01	0.06
11	131.4226	-8.39E+00	0.02
12	136.4327	-5.64E+00	0.01
13	137.7165	-3.35E+01	0.35
14	148.7184	-4.79E+00	0.01
15	155.8458	-4.77E+00	0.01
16	174.1687	-4.60E+00	0.01
17	186.9596	-4.21E+00	0.01
18	201.8193	3.78E+00	0.01
19	206.6192	4.11E+00	0.01
20	214.4651	-5.16E+00	0.01
21	239.1142	-1.90E+01	0.20
22	258.821	-5.85E+00	0.02
23	275.7784	3.32E+00	0.01
24	281.0366	1.71E+01	0.19
25	282.1662	6.92E+00	0.03
26	295.904	-6.09E+00	0.03
27	300.3628	-3.08E+00	0.01
28	327.1147	-4.52E+00	0.02
29	362.5773	3.19E+00	0.01
30	379.7033	2.64E+00	0.01
31	393.4667	7.39E+00	0.05
32	403.8377	1.03E+01	0.10
33	427.0024	-3.28E+00	0.01
34	435.2586	3.72E+00	0.01
35	448.9246	3.32E+00	0.01
36	457.0683	-3.24E+00	0.01
37	469.9991	-5.91E+00	0.04
38	483.433	-2.75E+00	0.01
39	488.712	9.12E+00	0.09

40	497.3784	2.11E+00	0.01
41	501.5825	-2.50E+00	0.01
42	506.4179	-4.84E+00	0.03
43	511.2945	-3.15E+00	0.01
44	514.0748	2.38E+00	0.01
45	548.7108	-3.36E+00	0.01
46	573.2549	5.27E+00	0.04
47	586.6248	2.46E+00	0.01
48	589.0658	-4.65E+00	0.03
49	597.8848	-1.78E+00	0.00
50	605.1359	-1.61E+00	0.00
51	607.1396	2.15E+00	0.01
52	612.6764	4.19E+00	0.02
53	624.9666	1.61E+00	0.00
54	636.7301	-8.19E+00	0.10
55	641.915	1.25E+00	0.00
56	651.5463	1.37E+00	0.00
57	654.3275	1.49E+00	0.00
58	666.4936	-2.15E+00	0.01
59	668.7696	-1.15E+00	0.00
60	677.715	1.38E+00	0.00
61	681.3229	-1.41E+00	0.00
62	693.6924	1.66E+00	0.00
63	699.8194	2.06E+00	0.01
64	704.8208	-1.56E+00	0.00
65	713.8814	1.07E+00	0.00
66	718.5379	-1.30E+00	0.00
67	722.3213	1.89E+00	0.01
68	728.3329	1.07E+00	0.00
69	742.5679	1.77E+00	0.01
70	744.4192	1.22E+00	0.00
71	747.5813	8.92E-01	0.00
72	749.4269	-2.46E+00	0.01
73	752.4201	-1.25E+00	0.00
74	757.9722	1.35E+00	0.00
75	758.2277	-2.96E+00	0.02
76	761.6585	1.13E+00	0.00
77	767.1129	1.30E+00	0.00
78	768.7016	1.23E+00	0.00
79	771.3231	-2.59E+00	0.01
80	775.0644	-1.00E+00	0.00
81	777.447	1.14E+00	0.00
82	778.3688	-1.05E+00	0.00
83	783.5113	1.03E+00	0.00
84	789.1361	1.07E+00	0.00
85	792.0541	-8.83E-01	0.00
86	799.3002	1.02E+00	0.00
87	804.32	1.30E+00	0.00
88	810.2072	1.62E+00	0.00
89	819.2041	-8.31E-01	0.00
90	821.2465	-7.08E-01	0.00

91	821.9884	1.17E+00	0.00
92	825.415	-1.08E+00	0.00
93	850.8431	7.93E-01	0.00
94	878.7285	-9.26E-01	0.00
95	893.2427	9.97E-01	0.00
96	900.9781	-1.04E+00	0.00
97	911.7432	-7.81E-01	0.00
98	913.9158	-7.55E-01	0.00
99	917.3997	-2.07E+00	0.01
100	930.1209	-6.10E-01	0.00
101	934.2309	-1.36E+00	0.00
102	938.682	-1.19E+00	0.00
103	942.3432	7.32E-01	0.00
104	944.8213	-6.84E-01	0.00
105	948.289	5.64E-01	0.00
106	950.6922	-1.04E+00	0.00
107	953.2269	5.85E-01	0.00
108	954.2841	7.24E-01	0.00
109	955.4802	-5.12E-01	0.00
110	956.9953	-6.02E-01	0.00
111	961.1678	9.53E-01	0.00
112	962.5578	6.26E-01	0.00
113	965.8372	4.68E-01	0.00
114	969.4191	-7.09E-01	0.00
115	971.8452	6.03E-01	0.00
116	973.0818	-4.77E-01	0.00
117	976.1474	-7.63E-01	0.00
118	981.0222	4.80E-01	0.00
119	981.7052	-4.50E-01	0.00
120	987.2827	4.58E-01	0.00
121	990.1129	2.88E-01	0.00
122	1006.0367	-9.03E-01	0.00
123	1008.4246	5.12E-01	0.00
124	1011.0018	4.82E-01	0.00
125	1016.0572	4.33E-01	0.00
126	1020.3087	-6.53E-01	0.00
127	1034.5041	8.05E-01	0.00
128	1037.4512	-4.74E-01	0.00
129	1038.6924	-4.84E-01	0.00
130	1045.4731	4.93E-01	0.00
131	1046.4241	3.67E-01	0.00
132	1052.8514	-5.15E-01	0.00
133	1057.5483	-4.52E-01	0.00
134	1064.69	-5.78E-01	0.00
135	1070.3989	3.81E-01	0.00
136	1077.8269	-2.01E-01	0.00
137	1091.2836	-4.55E-01	0.00
138	1096.3042	1.97E-01	0.00
139	1104.3429	-3.88E-01	0.00
140	1116.7075	-4.97E-01	0.00
141	1139.287	-4.33E-01	0.00

142	1149.585	-4.41E-01	0.00
143	1150.9692	-3.27E-01	0.00
144	1168.3219	3.23E-01	0.00
145	1170.2247	1.78E-01	0.00
146	1177.3958	-2.72E-01	0.00
147	1188.3999	-2.76E-01	0.00
148	1194.163	-1.66E-01	0.00
149	1194.9665	3.03E-01	0.00
150	1201.8381	-1.55E-01	0.00
151	1214.0002	2.84E-01	0.00
152	1282.7048	-2.56E-01	0.00
153	1296.8471	2.59E-01	0.00
154	1325.9203	-2.83E-01	0.00
155	1333.6742	2.81E-01	0.00
156	1340.4308	-2.76E-01	0.00
157	1346.9866	2.80E-01	0.00
158	1348.0501	2.43E-01	0.00
159	1356.5565	1.28E-01	0.00
160	1362.8418	1.88E-01	0.00
161	1369.5408	-1.81E-01	0.00
162	1380.8556	1.56E-01	0.00
163	1403.529	1.99E-01	0.00
164	1452.2614	-2.11E-01	0.00
165	1464.0678	-1.67E-01	0.00
166	1473.7954	-1.75E-01	0.00
167	1483.5739	9.45E-02	0.00
168	1488.8279	9.86E-02	0.00
169	1496.7746	1.49E-01	0.00
170	1511.6877	1.64E-01	0.00
171	1519.607	1.90E-01	0.00
172	1532.5881	1.43E-01	0.00
173	1544.8395	7.37E-02	0.00
174	1548.986	-1.24E-01	0.00
175	1562.1661	-6.43E-02	0.00
176	1594.9683	7.09E-02	0.00
177	1619.0892	1.10E-01	0.00
178	1625.767	1.10E-01	0.00
179	1647.3358	-1.34E-01	0.00
180	1649.5353	1.17E-01	0.00
181	1660.8043	1.01E-01	0.00
182	1683.7637	-6.12E-02	0.00
183	1690.8924	-1.27E-01	0.00
184	2686.9447	9.10E-02	0.00
185	2687.9885	-5.36E-02	0.00
186	2691.1245	-9.11E-02	0.00
187	2694.527	5.26E-02	0.00
188	2700.0839	-4.53E-02	0.00
189	2700.3443	7.69E-02	0.00
190	2709.2677	-3.63E-02	0.00
191	2716.0659	8.06E-02	0.00
192	2758.5359	-7.17E-02	0.00



193	2774.5168	-2.91E-02	0.00
194	3203.2953	2.41E-02	0.00
195	3210.1687	2.36E-02	0.00
196	3215.7948	1.99E-02	0.00
197	3217.6031	3.40E-02	0.00
198	3222.9188	3.63E-02	0.00
199	3227.754	-2.97E-02	0.00
200	3233.5471	-1.55E-02	0.00
201	3233.808	-1.66E-02	0.00
202	3236.8932	2.24E-02	0.00
203	3237.5843	-1.26E-02	0.00
204	3243.6212	-1.14E-02	0.00
205	3245.3823	-1.91E-02	0.00
206	3252.3708	-1.37E-02	0.00
207	3254.4437	-1.39E-02	0.00
208	3255.678	-5.34E-03	0.00
209	3257.4482	9.17E-03	0.00
210	3261.6921	4.85E-03	0.00
211	3268.082	3.54E-03	0.00
212	3273.5303	4.75E-04	0.00
213	3285.4446	-6.85E-05	0.00

**Table S6.** Vibrational frequencies ( $\omega_i/\text{cm}^{-1}$ ) at the respective optimized  $S_0$  states, Shift vector  $K_i$  (a.u.) and Huang-Rhys factor  $S_i$  of complex **2**

	$\omega_i/\text{cm}^{-1}$	$K_i$ (a.u.)	$S_i$
1	13.8489	-7.81E+01	0.19
2	20.8243	-1.76E+01	0.01
3	29.7386	-2.21E+02	3.33
4	34.9725	3.97E+01	0.13
5	36.1076	1.68E+01	0.02
6	44.2145	-8.62E+01	0.75
7	45.4383	-4.17E+01	0.18
8	54.73	-6.99E+01	0.61
9	60.9164	-1.83E+01	0.05
10	62.7697	-1.74E+01	0.04
11	70.9722	-6.50E+00	0.01
12	81.384	1.13E+01	0.02
13	95.7828	3.71E+01	0.30
14	105.3507	-3.82E+01	0.35
15	117.3025	-3.45E+01	0.32
16	124.712	-3.67E+01	0.38
17	136.8842	1.07E+01	0.04
18	138.0259	-4.11E+00	0.01
19	144.2533	-4.35E+00	0.01
20	152.4875	8.18E+00	0.02
21	160.6195	2.98E+01	0.33
22	164.4283	2.78E+01	0.29
23	182.8459	-2.71E+00	0.00
24	187.7173	-1.82E+01	0.14
25	202.3346	-9.52E+00	0.04

26	208.136	-4.72E+00	0.01
27	218.1257	-6.76E-01	0.00
28	229.1908	2.44E+01	0.31
29	236.7133	2.42E+01	0.32
30	250.7893	-4.87E+00	0.01
31	268.0486	-1.08E+01	0.07
32	277.6307	1.05E+01	0.07
33	281.3498	1.54E+00	0.00
34	286.8161	6.71E+00	0.03
35	302.9804	-1.19E+01	0.10
36	308.0735	-3.09E+00	0.01
37	322.9529	-9.20E+00	0.06
38	343.4681	4.01E+00	0.01
39	365.3081	-9.98E-01	0.00
40	391.2609	-6.60E+00	0.04
41	398.295	3.37E-01	0.00
42	412.8935	2.77E-01	0.00
43	417.81	3.76E-01	0.00
44	419.5192	2.01E+00	0.00
45	443.8572	3.58E-01	0.00
46	453.0928	1.69E+00	0.00
47	453.9277	-1.34E+00	0.00
48	465.4789	-1.95E+00	0.00
49	469.0447	-2.66E-01	0.00
50	476.9353	-4.49E+00	0.02
51	480.6001	-1.36E+00	0.00
52	483.21	-9.28E-01	0.00
53	493.0847	-2.70E+00	0.01
54	499.2742	4.47E+00	0.02
55	503.2696	3.72E+00	0.02
56	514.4664	3.93E-01	0.00
57	529.3858	-1.72E+00	0.00
58	543.9143	-2.43E+00	0.01
59	550.1239	1.26E-01	0.00
60	555.2146	1.21E+00	0.00
61	574.0587	5.59E-03	0.00
62	588.615	6.95E-01	0.00
63	589.3799	-2.62E+00	0.01
64	599.7656	1.14E+00	0.00
65	605.414	2.64E-01	0.00
66	607.6331	-2.71E-01	0.00
67	611.7628	2.20E+00	0.01
68	625.4479	1.31E+00	0.00
69	627.1044	-2.13E-01	0.00
70	627.3983	1.02E-02	0.00
71	636.9664	2.24E+00	0.01
72	638.0552	-1.99E+00	0.01
73	640.5265	-1.96E+00	0.01
74	653.9023	-1.10E-01	0.00
75	654.2578	-5.86E-01	0.00
76	667.6155	-7.47E-01	0.00

77	668.9455	-9.24E-01	0.00
78	673.6951	-1.07E+01	0.18
79	696.5342	2.66E+00	0.01
80	697.5532	9.25E-01	0.00
81	698.5298	8.41E-01	0.00
82	701.4015	-3.20E-01	0.00
83	704.4877	-1.41E+00	0.00
84	714.7916	5.54E-02	0.00
85	716.296	-1.01E-01	0.00
86	720.4428	-2.99E+00	0.01
87	726.7967	4.42E+00	0.03
88	730.8011	-2.07E-01	0.00
89	741.3661	-3.01E+00	0.02
90	743.1422	2.94E+00	0.01
91	748.0699	2.72E+00	0.01
92	749.8379	8.65E-01	0.00
93	754.5548	-4.94E-01	0.00
94	757.3561	9.91E-01	0.00
95	758.4468	5.15E-01	0.00
96	766.9776	5.55E-01	0.00
97	768.9658	-8.02E-01	0.00
98	771.134	-1.48E-02	0.00
99	772.9042	-6.04E-01	0.00
100	776.5362	-1.13E+00	0.00
101	778.7075	-2.43E+00	0.01
102	779.5704	-1.03E+00	0.00
103	780.9016	1.14E-01	0.00
104	787.6515	-3.82E-01	0.00
105	789.7314	-5.60E-01	0.00
106	793.1502	-1.36E+00	0.00
107	799.4049	1.96E-01	0.00
108	799.9867	-1.36E+00	0.00
109	803.6651	7.27E-01	0.00
110	811.2449	5.45E-02	0.00
111	812.1827	-2.29E+00	0.01
112	825.7196	-3.53E+00	0.02
113	831.7348	3.31E-01	0.00
114	836.1221	2.04E-01	0.00
115	842.8637	1.65E-01	0.00
116	849.6616	9.89E-01	0.00
117	850.6872	1.13E-02	0.00
118	863.956	1.73E-02	0.00
119	880.4744	-1.58E-01	0.00
120	896.1542	-3.95E-01	0.00
121	902.6749	-9.65E-01	0.00
122	912.6673	-1.28E-01	0.00
123	913.2878	8.27E-02	0.00
124	915.9545	1.00E-01	0.00
125	918.8811	-2.98E-01	0.00
126	927.0092	-1.16E+00	0.00
127	931.0814	1.52E-01	0.00

128	934.4459	5.80E-02	0.00
129	942.4388	-1.96E-01	0.00
130	943.4848	8.31E-02	0.00
131	947.3732	1.56E-01	0.00
132	948.2727	-7.20E-01	0.00
133	951.2645	-1.12E-01	0.00
134	953.858	1.27E+00	0.00
135	956.431	5.10E-02	0.00
136	957.4307	2.11E-01	0.00
137	961.09	3.02E-01	0.00
138	961.6112	-2.47E-01	0.00
139	963.6877	-5.12E-01	0.00
140	965.7679	-2.91E-01	0.00
141	967.8391	-2.81E-01	0.00
142	971.6561	-4.96E-01	0.00
143	973.3248	-7.14E-01	0.00
144	973.8876	1.94E-01	0.00
145	975.2642	-3.94E+00	0.03
146	978.6299	-6.75E+00	0.10
147	979.0691	-2.01E+00	0.01
148	983.1412	-1.94E+00	0.01
149	987.6365	-1.76E+00	0.01
150	990.0627	5.76E-01	0.00
151	993.6257	-6.55E-01	0.00
152	1002.724	-3.97E-01	0.00
153	1003.486	6.25E-02	0.00
154	1006.159	5.81E-01	0.00
155	1010.386	-1.10E+00	0.00
156	1016.489	4.49E-01	0.00
157	1019.733	-1.81E-02	0.00
158	1020.24	-4.30E+00	0.04
159	1030.603	4.12E-01	0.00
160	1035.531	1.10E+00	0.00
161	1039.511	5.55E+00	0.07
162	1042.037	-5.32E-01	0.00
163	1043.468	2.81E+00	0.02
164	1055.177	1.59E+00	0.01
165	1060.471	5.79E-02	0.00
166	1063.256	-3.01E+00	0.02
167	1065.787	5.98E-01	0.00
168	1070.696	-8.81E-01	0.00
169	1079.199	1.49E+00	0.01
170	1085.197	-7.61E-01	0.00
171	1091.542	-1.41E+00	0.00
172	1097.157	4.80E-01	0.00
173	1106.116	-1.07E+00	0.00
174	1117.123	-9.18E-02	0.00
175	1121.477	2.99E-01	0.00
176	1125.416	9.73E-02	0.00
177	1143.541	-8.24E-01	0.00
178	1149.951	-2.60E+00	0.02

179	1155.192	1.46E+00	0.01
180	1167.349	5.68E-02	0.00
181	1184.058	-5.96E-01	0.00
182	1187.184	-1.87E+00	0.01
183	1193.573	-1.62E+00	0.01
184	1193.878	8.38E-02	0.00
185	1195.63	-1.44E-02	0.00
186	1197.53	-8.63E-01	0.00
187	1217.928	-1.15E+00	0.00
188	1218.94	7.50E-02	0.00
189	1222.151	3.70E-01	0.00
190	1285.168	3.20E+00	0.03
191	1290.097	1.58E+00	0.01
192	1311.139	-1.33E-01	0.00
193	1321.313	7.55E-01	0.00
194	1332.325	-8.02E-02	0.00
195	1334.508	-1.98E+00	0.01
196	1334.893	2.16E+00	0.01
197	1342.03	-2.00E+00	0.01
198	1342.492	6.25E-02	0.00
199	1344.843	2.85E-01	0.00
200	1351.647	5.23E-01	0.00
201	1356.296	7.58E-02	0.00
202	1363.555	-1.58E+00	0.01
203	1371.915	2.00E+00	0.01
204	1379.537	1.96E+00	0.01
205	1386.093	4.90E+00	0.08
206	1390.202	-1.06E+00	0.00
207	1413.905	4.25E+00	0.06
208	1419.192	-4.05E+00	0.05
209	1440.687	3.39E+00	0.04
210	1464.379	2.45E+00	0.02
211	1479.281	9.66E-01	0.00
212	1485.807	-8.17E-01	0.00
213	1488.901	-5.00E-02	0.00
214	1492.576	2.00E+00	0.01
215	1503.839	-4.47E-02	0.00
216	1504.866	-6.33E-01	0.00
217	1517.813	-6.99E-01	0.00
218	1531.973	1.06E-01	0.00
219	1533.615	5.41E-01	0.00
220	1539.786	-9.56E-01	0.00
221	1545.538	1.56E+00	0.01
222	1558.172	-7.04E-01	0.00
223	1570.493	-4.55E-01	0.00
224	1614.088	3.69E+00	0.05
225	1619.323	-1.06E+00	0.00
226	1628.983	1.85E-03	0.00
227	1636.888	5.20E+00	0.10
228	1643.806	-4.57E-01	0.00
229	1649.936	2.55E+00	0.02

230	1661.378	1.05E+00	0.00
231	1661.615	1.54E-01	0.00
232	1669.48	-1.50E+00	0.01
233	1684.994	1.02E+00	0.00
234	1689.011	3.51E-01	0.00
235	1691.556	-4.76E-01	0.00
236	2684.822	1.87E-01	0.00
237	2687.175	4.75E-02	0.00
238	2687.768	-2.88E-02	0.00
239	2691.537	-6.27E-02	0.00
240	2697.388	-3.48E-02	0.00
241	2698.997	-5.43E-02	0.00
242	2708.1	-1.43E-01	0.00
243	2716.645	3.28E-01	0.00
244	2745.871	3.16E-02	0.00
245	2772.383	2.39E-01	0.00
246	3207.287	1.73E-01	0.00
247	3207.778	6.72E-03	0.00
248	3209.474	-1.10E-01	0.00
249	3212.32	-6.07E-02	0.00
250	3213.662	1.14E-02	0.00
251	3215.437	1.29E-01	0.00
252	3222.801	-1.29E-03	0.00
253	3227.453	1.85E-01	0.00
254	3229.18	2.70E-02	0.00
255	3229.289	1.32E-01	0.00
256	3231.03	-1.19E-02	0.00
257	3232.092	-1.17E-01	0.00
258	3232.984	2.70E-01	0.00
259	3234.187	-2.57E-01	0.00
260	3236.724	-6.00E-03	0.00
261	3238.442	-1.52E-01	0.00
262	3239.439	-3.72E-01	0.00
263	3241.054	-7.12E-03	0.00
264	3242.661	-8.53E-05	0.00
265	3245.364	-6.56E-02	0.00
266	3251.235	-9.54E-02	0.00
267	3253.78	1.36E-02	0.00
268	3257.583	3.56E-02	0.00
269	3258.968	-3.20E-02	0.00
270	3261.433	2.22E-01	0.00
271	3268.138	-1.62E-01	0.00
272	3279.744	-1.21E-02	0.00
273	3290.342	-1.88E-01	0.00

**Table S7.** Vibrational frequencies ( $\omega_i/\text{cm}^{-1}$ ) at the respective optimized  $S_0$  states, Shift vector  $K_i$  (a.u.) and Huang-Rhys factor  $S_i$  of complex **3**

	$\omega_i/\text{cm}^{-1}$	$K_i$ (a.u.)	$S_i$
1	30.1002	-5.86E+01	0.00
2	36.2584	7.33E+00	0.24

3	41.4948	2.55E+01	0.00
4	45.5458	-2.10E+01	0.06
5	52.4515	-4.24E+01	0.05
6	74.1741	-2.45E+01	0.22
7	87.4733	5.30E+00	0.10
8	96.3995	-4.84E+00	0.01
9	104.9912	-1.07E+01	0.01
10	127.7376	-8.38E+00	0.03
11	143.8101	-7.12E+00	0.02
12	153.4755	7.95E+00	0.02
13	161.7129	4.55E+00	0.02
14	174.52	3.83E+00	0.01
15	183.4935	-5.40E+00	0.01
16	190.0341	-8.89E-01	0.01
17	197.8738	6.52E+00	0.00
18	206.4985	1.23E+00	0.02
19	212.6815	8.59E+00	0.00
20	214.4511	7.83E+00	0.04
21	244.9653	1.52E+01	0.03
22	253.2294	1.57E+01	0.13
23	258.8675	1.73E+01	0.14
24	271.2656	-1.89E+01	0.18
25	281.7813	9.91E+00	0.22
26	286.7851	3.48E+00	0.06
27	299.1637	-1.70E+00	0.01
28	306.7217	-4.47E+00	0.00
29	335.8238	-1.82E+00	0.01
30	348.6789	2.96E+00	0.00
31	366.7516	2.19E+00	0.01
32	395.3815	-1.22E+00	0.00
33	435.2809	-1.61E+01	0.00
34	442.8808	-7.39E+00	0.26
35	447.3321	-5.14E-01	0.06
36	455.3022	1.45E+00	0.00
37	465.0325	1.21E-01	0.00
38	482.1385	1.07E-01	0.00
39	489.4559	1.24E+00	0.00
40	493.5277	3.27E+00	0.00
41	497.1419	3.86E+00	0.01
42	503.717	7.66E-01	0.02
43	514.6803	-5.09E-01	0.00
44	516.4644	4.38E-01	0.00
45	518.8382	-9.09E-02	0.00
46	525.0467	8.46E-01	0.00
47	543.02	3.14E+00	0.00
48	548.5369	8.22E-02	0.01
49	550.9286	-1.20E+00	0.00
50	562.1133	-2.72E+00	0.00
51	570.2107	-2.05E+00	0.01
52	584.512	-4.35E-01	0.01
53	589.0184	-1.64E+00	0.00

54	590.1832	-1.91E-01	0.00
55	598.7448	-3.51E-01	0.00
56	602.8407	-5.69E-01	0.00
57	605.295	-7.38E-01	0.00
58	606.8913	-6.07E-01	0.00
59	626.3652	5.03E-01	0.00
60	638.0432	3.63E-01	0.00
61	644.2835	-1.06E+00	0.00
62	655.9726	2.64E-02	0.00
63	660.3366	-2.59E+00	0.00
64	663.821	1.28E-01	0.01
65	666.3418	2.65E-01	0.00
66	677.1809	8.83E-01	0.00
67	700.0581	-6.69E-01	0.00
68	702.3025	9.32E-02	0.00
69	706.5904	4.93E-01	0.00
70	714.5558	8.94E-01	0.00
71	717.9609	-5.13E+00	0.00
72	727.6159	-2.87E-01	0.04
73	735.8004	1.78E-01	0.00
74	740.6407	-1.75E-01	0.00
75	746.1767	-1.76E-01	0.00
76	746.9336	5.47E-01	0.00
77	749.8342	-3.54E-01	0.00
78	751.299	-1.14E-01	0.00
79	753.0215	4.95E-01	0.00
80	758.3811	-3.39E-01	0.00
81	766.4339	2.78E-01	0.00
82	766.8786	-1.28E+00	0.00
83	768.5431	-2.10E-01	0.00
84	771.547	-3.94E-01	0.00
85	773.0682	4.23E-01	0.00
86	776.0176	-5.20E-01	0.00
87	777.7716	2.01E-01	0.00
88	781.6747	-5.26E-01	0.00
89	788.5083	4.62E-02	0.00
90	791.9787	1.31E-01	0.00
91	798.3168	-2.80E-01	0.00
92	803.5347	-2.11E-01	0.00
93	805.4633	-4.46E-01	0.00
94	807.1426	-4.66E-01	0.00
95	814.3566	1.07E-01	0.00
96	827.5355	2.92E-01	0.00
97	841.4884	-3.15E-01	0.00
98	855.0132	-7.47E-03	0.00
99	859.3246	-2.92E-01	0.00
100	861.641	4.57E-01	0.00
101	869.592	5.09E-01	0.00
102	876.0927	-2.93E-01	0.00
103	881.8697	-3.03E-01	0.00
104	890.1105	-1.09E+00	0.00



105	895.672	-1.10E+00	0.00
106	911.3791	-3.17E-02	0.00
107	916.3806	1.48E-02	0.00
108	918.3592	1.22E-01	0.00
109	929.448	-4.38E-01	0.00
110	930.7364	6.82E-02	0.00
111	933.0806	-5.55E-02	0.00
112	937.6733	-6.55E-02	0.00
113	940.5592	-4.45E-02	0.00
114	945.268	1.06E-01	0.00
115	946.622	5.95E-01	0.00
116	948.5805	-9.04E-02	0.00
117	950.8951	2.77E-01	0.00
118	952.7241	-3.66E-02	0.00
119	955.237	7.23E-02	0.00
120	955.9621	2.76E-02	0.00
121	958.9551	-2.37E+00	0.00
122	962.8052	-1.85E-01	0.01
123	965.6924	1.40E-01	0.00
124	969.2478	-1.39E-01	0.00
125	970.89	5.76E-01	0.00
126	977.1063	2.16E-02	0.00
127	979.8789	-2.80E-01	0.00
128	981.2736	-2.49E-01	0.00
129	986.9871	-3.98E-01	0.00
130	991.4181	-1.80E-02	0.00
131	994.0298	2.28E-01	0.00
132	997.6245	1.27E+00	0.00
133	1006.325	-2.73E-02	0.00
134	1012.276	-1.64E-01	0.00
135	1019.717	3.67E-02	0.00
136	1036.325	2.87E-01	0.00
137	1041.623	1.36E+00	0.00
138	1045.927	-5.68E-01	0.00
139	1054.077	-4.02E+00	0.00
140	1065.572	2.63E-01	0.04
141	1078.166	9.11E-01	0.00
142	1092.06	1.06E-01	0.00
143	1099.467	5.82E-01	0.00
144	1104.568	5.80E+00	0.00
145	1117.222	-2.76E-01	0.08
146	1119.351	-6.13E-01	0.00
147	1120.237	-1.52E+00	0.00
148	1124.639	1.56E+00	0.01
149	1140.421	-3.28E+00	0.01
150	1146.622	3.66E+00	0.03
151	1151.386	-2.47E-01	0.04
152	1178.537	-1.79E-01	0.00
153	1187.668	2.25E-01	0.00
154	1195.444	-6.46E-03	0.00
155	1205.733	2.30E+00	0.00

156	1211.62	-2.19E+00	0.01
157	1230.144	-2.85E+00	0.01
158	1237.309	-3.16E+00	0.02
159	1241.912	-2.14E+00	0.03
160	1257.089	1.23E-01	0.01
161	1264.236	9.85E-02	0.00
162	1280.057	2.33E-02	0.00
163	1334.57	-3.22E-01	0.00
164	1343.5	6.85E-01	0.00
165	1345.467	1.53E+00	0.00
166	1346.934	1.93E+00	0.01
167	1355.716	3.35E+00	0.01
168	1369.101	-6.51E-01	0.03
169	1373.536	-5.69E+00	0.00
170	1376.174	1.01E+01	0.10
171	1411.856	1.11E-02	0.32
172	1427.883	2.86E+00	0.00
173	1447.359	-1.55E+00	0.03
174	1456.045	-5.79E-02	0.01
175	1464.461	-1.30E-01	0.00
176	1468.529	-4.61E+00	0.00
177	1481.675	-8.46E-02	0.07
178	1488.352	-4.46E+00	0.00
179	1490.865	5.16E-01	0.07
180	1502.78	-2.33E+00	0.00
181	1509.011	-9.66E-02	0.02
182	1517.21	2.90E+00	0.00
183	1535.763	-3.62E-03	0.03
184	1546.425	-4.86E+00	0.00
185	1553.662	5.05E-01	0.08
186	1557.808	-2.47E-01	0.00
187	1570.156	1.29E-01	0.00
188	1577.604	1.52E-01	0.00
189	1621.358	8.55E+00	0.00
190	1642.494	3.58E-01	0.27
191	1651.545	3.52E-01	0.00
192	1654.226	4.26E-01	0.00
193	1674.052	1.22E-01	0.00
194	1687.244	5.53E-02	0.00
195	1699.179	2.34E-01	0.00
196	2684.025	2.31E-02	0.00
197	2686.79	-1.24E-03	0.00
198	2687.893	1.12E-02	0.00
199	2693.682	-2.40E-02	0.00
200	2698.316	-8.73E-03	0.00
201	2699.899	-1.97E-02	0.00
202	2708.959	2.75E-02	0.00
203	2721.854	-5.40E-02	0.00
204	2736.04	1.20E-02	0.00
205	2779.542	-8.43E-02	0.00
206	3203.71	-8.58E-03	0.00

207	3208.366	9.06E-03	0.00
208	3209.688	5.30E-02	0.00
209	3211.999	4.73E-02	0.00
210	3221.192	3.84E-02	0.00
211	3221.736	9.48E-03	0.00
212	3224.338	-2.34E-01	0.00
213	3226.7	2.58E-02	0.00
214	3227.482	-9.62E-03	0.00
215	3228.915	-5.02E-02	0.00
216	3234.619	-5.60E-02	0.00
217	3234.926	7.35E-03	0.00
218	3240.847	-1.25E-01	0.00
219	3250.65	1.45E-01	0.00
220	3251.798	1.16E-02	0.00
221	3253.39	6.55E-04	0.00
222	3265.714	-2.56E-02	0.00
223	3267.87	2.10E-02	0.00
224	3287.668	1.41E-01	0.00
225	3300.785	-1.60E-02	0.00

**Table S8.** Vibrational frequencies ( $\omega_i/\text{cm}^{-1}$ ) at the respective optimized  $S_0$  states, Shift vector  $K_i$  (a.u.) and Huang-Rhys factor  $S_i$  of complex **3a**

	$\omega_i/\text{cm}^{-1}$	$K_i$ (a.u.)	$S_i$
1	295.0107	-2.45E+01	1.16
2	67.4739	-4.42E+01	0.78
3	241.5628	-1.70E+01	0.44
4	286.7812	-1.46E+01	0.40
5	148.608	1.99E+01	0.30
6	221.7475	1.54E+01	0.16
7	410.169	-1.13E+01	0.14
8	1069.599	-6.72E+00	0.13
9	66.7275	-2.56E+01	0.12
10	96.8396	-2.10E+01	0.12
11	195.7654	-1.44E+01	0.11
12	300.9421	-1.05E+01	0.10
13	303.5613	-1.01E+01	0.10
14	99.8193	-1.61E+01	0.09
15	63.693	-1.97E+01	0.08
16	932.9171	-5.02E+00	0.07
17	1135.695	-4.53E+00	0.06
18	121.2483	1.36E+01	0.06
19	32.6977	-2.57E+01	0.05
20	23.5918	-2.96E+01	0.05
21	87.2621	1.53E+01	0.05
22	280.8298	8.18E+00	0.05
23	1032.019	-4.22E+00	0.05
24	453.9388	-6.32E+00	0.05
25	187.7685	9.71E+00	0.04
26	332.1383	-7.28E+00	0.04
27	134.2809	-1.10E+01	0.04

28	231.2397	-8.26E+00	0.04
29	678.2139	-4.33E+00	0.04
30	927.4315	3.67E+00	0.04
31	276.2508	-6.64E+00	0.04
32	924.0057	3.59E+00	0.03
33	499.6407	-4.83E+00	0.03
34	1294.673	2.90E+00	0.03
35	595.7828	-4.21E+00	0.03
36	1642.471	2.50E+00	0.03
37	446.9465	4.68E+00	0.02
38	322.4035	5.39E+00	0.02
39	636.876	3.82E+00	0.02
40	441.0479	-4.51E+00	0.02
41	1660.108	-2.30E+00	0.02
42	1546.882	2.35E+00	0.02
43	751.091	3.28E+00	0.02
44	1310.759	2.44E+00	0.02
45	548.8571	-3.75E+00	0.02
46	439.1483	-4.14E+00	0.02
47	365.9619	4.52E+00	0.02
48	642.1056	-3.39E+00	0.02
49	1261.292	2.40E+00	0.02
50	748.471	3.07E+00	0.02
51	1387.571	-2.25E+00	0.02
52	181.9246	6.15E+00	0.02
53	1413.53	2.21E+00	0.02
54	660.7224	-3.19E+00	0.02
55	425.9961	3.55E+00	0.02
56	152.2284	5.93E+00	0.02
57	472.585	-3.36E+00	0.02
58	1124.864	2.15E+00	0.01
59	1076.225	2.19E+00	0.01
60	637.8374	2.62E+00	0.01
61	1095.538	-1.89E+00	0.01
62	1231.348	1.78E+00	0.01
63	1051.484	-1.90E+00	0.01
64	1187.012	1.73E+00	0.01
65	444.4407	2.73E+00	0.01
66	1208.625	-1.65E+00	0.01
67	745.596	2.09E+00	0.01
68	165.8938	4.27E+00	0.01
69	268.632	3.31E+00	0.01
70	496.0889	2.41E+00	0.01
71	1041.213	-1.66E+00	0.01
72	596.9628	2.19E+00	0.01
73	1574.346	1.35E+00	0.01
74	1393.865	-1.41E+00	0.01
75	125.9753	-4.67E+00	0.01
76	1085.951	-1.57E+00	0.01
77	759.8434	1.80E+00	0.01
78	811.4927	-1.73E+00	0.01

79	735.2569	-1.81E+00	0.01
80	942.5934	1.59E+00	0.01
81	432.2508	-2.34E+00	0.01
82	1239.997	-1.38E+00	0.01
83	614.5823	1.96E+00	0.01
84	941.5909	1.57E+00	0.01
85	1092.924	-1.44E+00	0.01
86	606.8339	-1.86E+00	0.01
87	1496.302	1.18E+00	0.01
88	40.6889	-6.98E+00	0.01
89	603.0984	1.80E+00	0.00
90	203.0875	3.09E+00	0.00
91	1168.867	-1.27E+00	0.00
92	320.795	-2.36E+00	0.00
93	938.1488	1.36E+00	0.00
94	1483.784	1.06E+00	0.00
95	1344.279	1.07E+00	0.00
96	918.315	1.25E+00	0.00
97	806.3875	-1.31E+00	0.00
98	951.2053	1.19E+00	0.00
99	906.3255	1.20E+00	0.00
100	622.2571	-1.44E+00	0.00
101	1285.703	-1.00E+00	0.00
102	774.3338	-1.27E+00	0.00
103	590.0596	-1.43E+00	0.00
104	1457.462	9.01E-01	0.00
105	1401.436	9.18E-01	0.00
106	1126.491	1.02E+00	0.00
107	1488.855	-8.67E-01	0.00
108	871.2767	-1.11E+00	0.00
109	1648.827	8.03E-01	0.00
110	1516.411	-8.34E-01	0.00
111	1377.219	-8.75E-01	0.00
112	943.8842	1.04E+00	0.00
113	1368.723	-8.63E-01	0.00
114	1164.418	-9.27E-01	0.00
115	829.1535	1.09E+00	0.00
116	1679.585	-7.59E-01	0.00
117	456.4967	-1.45E+00	0.00
118	746.9039	-1.14E+00	0.00
119	1490.434	7.88E-01	0.00
120	669.7687	1.16E+00	0.00
121	1436.731	7.79E-01	0.00
122	630.0488	-1.18E+00	0.00
123	1191.916	8.30E-01	0.00
124	557.2335	1.18E+00	0.00
125	699.401	-1.01E+00	0.00
126	987.8197	-8.48E-01	0.00
127	726.0166	-9.82E-01	0.00
128	568.3009	1.09E+00	0.00
129	1032.316	-7.90E-01	0.00

130	1651.003	6.23E-01	0.00
131	954.5128	8.14E-01	0.00
132	1140.691	-7.44E-01	0.00
133	706.9553	9.34E-01	0.00
134	546.9114	1.06E+00	0.00
135	435.4251	-1.19E+00	0.00
136	807.279	-8.57E-01	0.00
137	948.3238	7.82E-01	0.00
138	483.5661	1.07E+00	0.00
139	752.9096	-8.54E-01	0.00
140	740.331	-8.12E-01	0.00
141	1132.084	-6.54E-01	0.00
142	952.8112	7.00E-01	0.00
143	815.5404	7.43E-01	0.00
144	1155.852	6.11E-01	0.00
145	924.4235	6.81E-01	0.00
146	770.4145	-7.37E-01	0.00
147	1479.024	5.25E-01	0.00
148	709.0307	7.46E-01	0.00
149	665.4083	7.59E-01	0.00
150	1035.869	-5.91E-01	0.00
151	1556.549	4.81E-01	0.00
152	1018.654	-5.92E-01	0.00
153	1609.271	4.69E-01	0.00
154	651.2449	-6.55E-01	0.00
155	818.7376	-5.74E-01	0.00
156	1407.579	4.21E-01	0.00
157	850.0842	5.31E-01	0.00
158	598.7719	-6.26E-01	0.00
159	790.5067	5.40E-01	0.00
160	1304.184	-4.03E-01	0.00
161	967.224	-4.63E-01	0.00
162	797.4089	-5.03E-01	0.00
163	481.2948	6.39E-01	0.00
164	1117.832	4.08E-01	0.00
165	1430.773	3.56E-01	0.00
166	1624.603	3.02E-01	0.00
167	1353.237	-3.18E-01	0.00
168	864.4212	-3.97E-01	0.00
169	937.1147	-3.65E-01	0.00
170	757.7673	4.00E-01	0.00
171	3264.955	-1.93E-01	0.00
172	1353.915	2.98E-01	0.00
173	1064.47	3.33E-01	0.00
174	826.1774	-3.75E-01	0.00
175	1113.201	-3.13E-01	0.00
176	1599.583	-2.55E-01	0.00
177	625.855	4.01E-01	0.00
178	766.8797	3.58E-01	0.00
179	1541.131	-2.50E-01	0.00
180	1200.981	-2.82E-01	0.00

181	514.0225	-4.27E-01	0.00
182	3226.423	1.69E-01	0.00
183	1151.449	-2.81E-01	0.00
184	1690.993	-2.27E-01	0.00
185	800.2405	-3.23E-01	0.00
186	605.8693	-3.71E-01	0.00
187	767.7459	-3.17E-01	0.00
188	999.2151	2.77E-01	0.00
189	1001.688	-2.76E-01	0.00
190	587.8721	3.51E-01	0.00
191	714.3064	3.16E-01	0.00
192	773.7202	-2.81E-01	0.00
193	3224.803	-1.35E-01	0.00
194	139.0875	6.25E-01	0.00
195	1333.584	1.97E-01	0.00
196	881.5884	-2.38E-01	0.00
197	3246.97	1.21E-01	0.00
198	910.8383	-2.27E-01	0.00
199	754.7852	-2.40E-01	0.00
200	1678.229	-1.56E-01	0.00
201	1533.35	-1.62E-01	0.00
202	835.5969	-2.16E-01	0.00
203	989.388	1.98E-01	0.00
204	3245.305	-9.89E-02	0.00
205	1195.591	1.62E-01	0.00
206	980.6829	1.73E-01	0.00
207	3217.838	9.45E-02	0.00
208	3251.23	9.21E-02	0.00
209	1346.962	1.43E-01	0.00
210	1536.1	-1.33E-01	0.00
211	1039.868	1.58E-01	0.00
212	839.4854	1.66E-01	0.00
213	3255.193	8.41E-02	0.00
214	1019.2	-1.48E-01	0.00
215	3236.129	7.81E-02	0.00
216	965.6961	-1.32E-01	0.00
217	2783.763	-7.73E-02	0.00
218	3236.182	7.12E-02	0.00
219	961.8188	-1.27E-01	0.00
220	1508.061	-1.00E-01	0.00
221	857.7041	1.29E-01	0.00
222	762.3524	-1.27E-01	0.00
223	980.9537	-1.12E-01	0.00
224	2744.116	6.62E-02	0.00
225	974.7183	1.01E-01	0.00
226	990.5299	-1.00E-01	0.00
227	581.3372	1.20E-01	0.00
228	3278.163	4.83E-02	0.00
229	955.8336	-8.91E-02	0.00
230	2726.251	-5.15E-02	0.00
231	3244.542	4.72E-02	0.00

232	3217.523	3.83E-02	0.00
233	789.7311	7.71E-02	0.00
234	951.761	6.69E-02	0.00
235	787.259	6.47E-02	0.00
236	1340.795	-4.73E-02	0.00
237	3274.168	-2.84E-02	0.00
238	3246.453	-2.20E-02	0.00
239	2711.358	2.32E-02	0.00
240	3294.938	1.74E-02	0.00
241	3258.351	1.65E-02	0.00
242	2688.734	-1.69E-02	0.00
243	2691.153	-1.57E-02	0.00
244	3228.38	-1.39E-02	0.00
245	913.8108	-2.49E-02	0.00
246	3211.353	1.30E-02	0.00
247	2700.59	1.38E-02	0.00
248	3212.966	-1.09E-02	0.00
249	976.3672	1.95E-02	0.00
250	3267.67	9.28E-03	0.00
251	3240.381	9.08E-03	0.00
252	2687.224	-8.95E-03	0.00
253	1614.656	1.04E-02	0.00
254	2702.682	-6.60E-03	0.00
255	3253.334	1.68E-03	0.00
256	777.9098	-2.26E-03	0.00
257	3235.467	2.90E-04	0.00
258	2696.621	2.24E-04	0.00
259	295.0107	-2.45E+01	0.00
260	67.4739	-4.42E+01	0.00
261	241.5628	-1.70E+01	0.00

**Table S9.** Vibrational frequencies ( $\omega_i/\text{cm}^{-1}$ ) at the respective optimized  $S_0$  states, Shift vector  $K_i$  (a.u.) and Huang-Rhys factor  $S_i$  of complex **4**.

	$\omega_i/\text{cm}^{-1}$	$K_i$ (a.u.)	$S_i$
1	20.0013	-2.28E+01	0.02
2	29.3166	-3.14E+01	0.07
3	38.1412	1.80E+00	0.00
4	38.4779	-4.09E+00	0.00
5	41.7552	3.62E-01	0.00
6	59.6003	9.63E+00	0.01
7	62.0977	-9.59E+00	0.01
8	68.4931	-6.31E+00	0.01
9	87.2788	-4.71E+00	0.00
10	94.7923	5.21E+00	0.01
11	112.1342	-1.20E+01	0.04
12	114.5182	-2.62E+01	0.18
13	131.3649	8.47E-01	0.00
14	135.3877	1.13E+01	0.04
15	137.992	9.58E+00	0.03
16	148.9397	4.61E-01	0.00



17	155.7571	1.44E+01	0.07
18	160.5785	9.49E+00	0.03
19	167.8646	-8.49E+00	0.03
20	190.9832	5.06E+00	0.01
21	204.0692	-2.34E+00	0.00
22	208.861	-7.56E+00	0.03
23	221.5072	2.17E+00	0.00
24	233.2944	-6.91E+00	0.03
25	243.3251	9.44E+00	0.05
26	267.1311	2.98E+00	0.01
27	271.7108	-5.72E+00	0.02
28	278.5223	-1.98E+00	0.00
29	281.7039	-1.60E+00	0.00
30	282.9426	-7.93E-01	0.00
31	303.7413	-7.20E-02	0.00
32	313.6214	-7.61E+00	0.04
33	321.5169	9.41E+00	0.07
34	326.078	5.56E+00	0.02
35	361.8633	2.77E+00	0.01
36	368.4896	-5.17E+00	0.02
37	375.6911	3.32E+00	0.01
38	384.7988	-1.10E+01	0.11
39	409.4135	-6.36E-03	0.00
40	426.9553	-1.67E+00	0.00
41	450.6092	-2.60E+00	0.01
42	466.1707	-6.95E-01	0.00
43	473.6957	-8.76E-01	0.00
44	483.5958	8.64E-02	0.00
45	484.9712	3.67E-02	0.00
46	497.5867	1.55E+00	0.00
47	513.4323	1.46E+00	0.00
48	515.2629	-1.62E-01	0.00
49	525.6638	8.10E-01	0.00
50	529.9712	-7.72E-02	0.00
51	532.8102	-1.67E+00	0.00
52	538.9401	9.54E+00	0.11
53	550.1912	1.31E+00	0.00
54	562.5265	-9.32E-01	0.00
55	568.9187	1.53E-01	0.00
56	572.1843	-6.68E-01	0.00
57	588.8435	5.09E-01	0.00
58	591.104	1.38E+00	0.00
59	597.1005	7.17E+00	0.07
60	599.497	-2.06E+00	0.01
61	599.9782	9.39E-01	0.00
62	604.6074	-3.38E-01	0.00
63	607.1646	-6.64E-01	0.00
64	625.7553	-8.65E-02	0.00
65	630.785	-4.99E+00	0.04
66	638.3629	1.79E-01	0.00
67	650.5289	-8.02E-01	0.00

68	650.9766	-1.10E+00	0.00
69	655.5361	-5.39E-01	0.00
70	663.3166	1.26E-01	0.00
71	668.1361	1.56E-01	0.00
72	674.6508	-1.26E+00	0.00
73	701.4218	1.26E-01	0.00
74	702.2067	-2.12E-01	0.00
75	705.2051	-2.23E-01	0.00
76	714.6163	4.57E-01	0.00
77	717.346	-9.25E-01	0.00
78	728.4279	-3.68E-01	0.00
79	732.7128	-2.12E-01	0.00
80	735.8022	1.30E+00	0.00
81	741.1609	-4.57E-02	0.00
82	742.0678	2.64E-01	0.00
83	744.4076	9.34E-01	0.00
84	748.602	-1.87E-01	0.00
85	750.8112	-1.59E-01	0.00
86	752.9329	-5.85E-01	0.00
87	758.2959	-1.09E-01	0.00
88	761.6473	2.60E-01	0.00
89	766.6617	1.90E-01	0.00
90	769.0453	-8.19E-02	0.00
91	773.1097	-2.07E-01	0.00
92	773.8706	-1.21E-02	0.00
93	777.0375	-4.53E-01	0.00
94	779.0009	8.64E-03	0.00
95	785.2721	1.42E-01	0.00
96	786.1856	5.51E-02	0.00
97	789.4492	1.86E-01	0.00
98	793.5832	4.92E-01	0.00
99	799.9565	-7.59E-01	0.00
100	801.7434	-2.75E+00	0.01
101	804.4071	8.70E-01	0.00
102	809.0876	-2.15E-02	0.00
103	809.7253	-4.37E-01	0.00
104	816.7829	-3.77E-01	0.00
105	820.9703	-3.96E-01	0.00
106	826.8842	3.11E-01	0.00
107	851.5176	-2.23E-01	0.00
108	853.8864	-1.07E-01	0.00
109	866.3906	9.96E-03	0.00
110	867.9896	1.81E-01	0.00
111	880.0587	-1.62E-01	0.00
112	892.1452	-2.91E+00	0.02
113	897.6808	-1.01E-01	0.00
114	898.6522	2.41E-01	0.00
115	904.0217	-1.27E-01	0.00
116	905.3175	-1.94E-02	0.00
117	912.577	2.98E-03	0.00
118	917.1247	-4.19E-02	0.00

119	919.5111	-4.42E-02	0.00
120	931.0457	1.38E-01	0.00
121	935.1896	-2.63E-01	0.00
122	935.7129	-1.22E-01	0.00
123	941.6842	-6.05E-02	0.00
124	947.1169	-4.07E-02	0.00
125	948.2382	-5.78E-03	0.00
126	950.9975	-1.68E-01	0.00
127	953.4913	-1.37E-02	0.00
128	955.8577	-6.42E-02	0.00
129	957.2916	-4.18E-02	0.00
130	963.8051	-2.01E-02	0.00
131	964.1373	-1.95E-02	0.00
132	966.2986	-2.05E-01	0.00
133	967.4615	8.29E-02	0.00
134	967.7707	-7.83E-03	0.00
135	970.3923	-1.51E+00	0.01
136	974.9638	-9.01E-02	0.00
137	976.0329	-4.92E-02	0.00
138	980.2461	8.22E-03	0.00
139	983.3381	-1.27E-01	0.00
140	985.0801	8.23E-02	0.00
141	989.3207	3.94E-02	0.00
142	993.229	3.88E-02	0.00
143	997.8984	1.94E-02	0.00
144	1003.778	6.12E-02	0.00
145	1019.771	-1.00E-01	0.00
146	1020.557	3.84E-02	0.00
147	1026.749	1.24E-01	0.00
148	1035.861	-1.91E-01	0.00
149	1042.199	-6.45E-01	0.00
150	1043.01	-1.08E+00	0.00
151	1050.371	6.79E-01	0.00
152	1061.436	3.18E-02	0.00
153	1066.039	-9.87E-02	0.00
154	1077.244	-2.90E+00	0.02
155	1079.29	3.46E+00	0.03
156	1085.939	2.00E+00	0.01
157	1086.486	-2.68E+00	0.02
158	1093.115	-3.13E-01	0.00
159	1105.642	-2.43E-01	0.00
160	1111.092	9.37E-01	0.00
161	1117.775	-1.61E-01	0.00
162	1148.603	4.06E-01	0.00
163	1151.139	-1.53E-01	0.00
164	1154.315	-1.49E-01	0.00
165	1170.936	-1.16E+00	0.00
166	1171.896	-2.36E+00	0.01
167	1179.57	-7.93E-01	0.00
168	1189.544	-5.17E-01	0.00
169	1192.362	2.05E+00	0.01

170	1194.378	-9.21E-02	0.00
171	1196.135	-4.63E-02	0.00
172	1212.567	-2.99E+00	0.02
173	1247.475	2.52E-01	0.00
174	1248.554	-3.65E-01	0.00
175	1262.417	-3.53E-03	0.00
176	1303.764	2.11E-01	0.00
177	1307.324	2.71E-01	0.00
178	1313.416	7.82E-01	0.00
179	1323.105	4.08E+00	0.05
180	1335.948	1.90E-01	0.00
181	1338.801	3.06E+00	0.03
182	1342.274	-6.03E+00	0.11
183	1344.553	-3.46E-01	0.00
184	1345.547	5.09E-01	0.00
185	1350.609	-5.65E-01	0.00
186	1368.568	1.36E+00	0.01
187	1373.792	3.17E-01	0.00
188	1396.514	7.09E+00	0.16
189	1425.365	-2.62E-01	0.00
190	1426.056	8.90E-01	0.00
191	1447.169	-6.64E+00	0.15
192	1451.466	8.52E-02	0.00
193	1475.112	-1.35E-01	0.00
194	1487.36	2.85E+00	0.03
195	1490.153	1.61E-02	0.00
196	1493.869	1.29E+00	0.01
197	1494.551	-4.31E+00	0.06
198	1506.819	-6.68E-01	0.00
199	1511.391	2.99E+00	0.03
200	1530.123	-4.23E+00	0.06
201	1535.188	-2.06E-01	0.00
202	1536.814	-1.35E-01	0.00
203	1547.866	-8.54E+00	0.26
204	1558.416	-8.64E-02	0.00
205	1566.438	-2.35E+00	0.02
206	1603.576	1.19E+00	0.01
207	1634.837	-4.34E+00	0.07
208	1639.693	-1.11E-01	0.00
209	1645.148	-8.05E-02	0.00
210	1650.968	4.79E-02	0.00
211	1664.501	3.27E-01	0.00
212	1677.008	5.69E+00	0.12
213	1686.62	-1.23E-01	0.00
214	1690.531	2.14E-01	0.00
215	1703.976	-5.50E-02	0.00
216	2682.204	3.41E-02	0.00
217	2686.363	-8.38E-03	0.00
218	2687.157	9.11E-03	0.00
219	2692.286	-1.97E-02	0.00
220	2697.24	-1.86E-02	0.00

221	2699.122	-8.66E-03	0.00
222	2708.043	-1.51E-03	0.00
223	2721.354	-6.37E-02	0.00
224	2734.896	-1.10E-03	0.00
225	2782.735	-1.06E-01	0.00
226	3198.956	2.21E-03	0.00
227	3202.396	-7.40E-05	0.00
228	3205.472	-7.30E-02	0.00
229	3207.986	-2.72E-03	0.00
230	3209.856	1.30E-02	0.00
231	3213.278	-4.03E-02	0.00
232	3217.417	-2.47E-01	0.00
233	3222.975	1.34E-02	0.00
234	3224.689	2.37E-02	0.00
235	3225.39	7.00E-02	0.00
236	3230.878	3.75E-03	0.00
237	3233.975	1.34E-01	0.00
238	3234.819	-1.53E-03	0.00
239	3236.384	-4.57E-03	0.00
240	3242.752	5.64E-02	0.00
241	3250.264	6.44E-03	0.00
242	3251.244	5.89E-02	0.00
243	3255.245	-5.92E-02	0.00
244	3255.325	5.17E-03	0.00
245	3260.128	1.70E-04	0.00
246	3262.151	-1.38E-02	0.00
247	3268.025	3.38E-03	0.00
248	3272.768	-1.51E-02	0.00
249	3302.123	-1.57E-02	0.00

Table S10. Vibrational frequencies ( $\omega_i/\text{cm}^{-1}$ ) at the respective optimized  $S_0$  states, Shift vector  $K_i$  (a.u.) and Huang-Rhys factor  $S_i$  of complex **4a**.

	$\omega_i/\text{cm}^{-1}$	$K_i$ (a.u.)	$S_i$
1	20.8587	-1.20E+02	0.69
2	31.9226	-1.98E+02	2.87
3	35.7541	6.06E+01	0.30
4	36.7299	5.21E+01	0.23
5	41.8632	1.48E+02	2.08
6	60.1927	-3.08E+01	0.13
7	66.2627	1.30E+01	0.03
8	79.4682	9.39E+01	1.60
9	84.3987	3.15E+01	0.19
10	98.2619	2.52E+01	0.14
11	109.9889	9.82E+00	0.02
12	119.7078	-3.61E+01	0.36
13	130.321	-3.58E+01	0.38
14	137.9189	4.47E+00	0.01
15	138.8376	5.68E+00	0.01
16	159.8502	-7.70E+00	0.02
17	162.411	2.80E+00	0.00

18	168.891	1.47E+00	0.00
19	181.5982	3.44E+00	0.00
20	191.7028	-3.76E+00	0.01
21	200.5543	1.32E+00	0.00
22	206.0669	1.08E+00	0.00
23	220.8655	9.01E-01	0.00
24	225.2167	4.21E+00	0.01
25	237.0236	-3.66E+00	0.01
26	260.3666	5.79E+00	0.02
27	279.0149	1.15E+01	0.08
28	279.9245	5.18E+00	0.02
29	283.7357	-4.63E+00	0.01
30	298.6875	4.30E+00	0.01
31	304.173	2.66E+00	0.00
32	319.6998	9.42E-01	0.00
33	348.5531	-4.28E+00	0.01
34	358.2267	2.14E+00	0.00
35	362.4844	9.80E-01	0.00
36	368.3437	-4.55E-01	0.00
37	373.3121	2.71E+00	0.01
38	404.4631	-1.55E+00	0.00
39	420.897	-7.58E-01	0.00
40	442.5217	-7.34E+00	0.05
41	454.0951	4.52E+00	0.02
42	475.5108	9.96E-01	0.00
43	478.7524	8.51E-01	0.00
44	482.2714	9.88E-03	0.00
45	486.7302	1.42E+00	0.00
46	495.4258	4.86E-01	0.00
47	498.1545	-5.85E-01	0.00
48	512.9558	-2.10E+00	0.01
49	515.6197	2.78E-02	0.00
50	518.9831	1.65E+01	0.32
51	531.5728	-2.49E+00	0.01
52	536.6173	1.46E+01	0.26
53	538.5907	1.72E+01	0.37
54	548.3231	-6.55E-01	0.00
55	550.1549	5.44E-02	0.00
56	584.4123	9.22E-01	0.00
57	587.7161	3.49E-02	0.00
58	592.1121	8.51E-02	0.00
59	598.9092	4.09E-01	0.00
60	603.2665	-2.07E-01	0.00
61	605.8532	-1.01E-01	0.00
62	613.6767	-5.15E+00	0.04
63	615.0102	-1.26E+00	0.00
64	624.7822	-1.37E-01	0.00
65	632.9205	-1.39E+00	0.00
66	636.4731	-3.48E-01	0.00
67	648.0878	2.11E-01	0.00
68	654.1962	1.79E+00	0.00

69	661.9387	4.66E+00	0.03
70	664.8316	3.27E+00	0.02
71	669.5236	9.94E-01	0.00
72	672.708	1.55E+00	0.00
73	695.3951	1.54E+00	0.00
74	701.9135	-7.69E-01	0.00
75	703.8366	6.79E-01	0.00
76	712.2522	9.78E+00	0.16
77	714.6899	1.07E+00	0.00
78	722.1307	-1.43E+01	0.34
79	726.2652	9.55E-01	0.00
80	731.3615	-8.38E-01	0.00
81	740.9379	-3.27E-01	0.00
82	743.9386	3.98E+00	0.03
83	746.273	5.43E-01	0.00
84	750.549	1.87E-01	0.00
85	755.2402	-2.25E+00	0.01
86	757.4476	2.30E-01	0.00
87	763.68	3.36E-01	0.00
88	766.0846	1.77E-01	0.00
89	769.7918	-1.33E-01	0.00
90	771.8795	-1.22E+00	0.00
91	772.4151	-4.38E-01	0.00
92	776.0403	-4.29E-01	0.00
93	777.7288	8.18E-02	0.00
94	783.5315	1.35E-01	0.00
95	788.1313	2.60E-01	0.00
96	789.1005	-3.85E-01	0.00
97	790.8031	8.06E-02	0.00
98	792.8714	3.41E-01	0.00
99	798.3908	-2.98E-01	0.00
100	800.7755	-9.52E-02	0.00
101	811.2117	1.96E-01	0.00
102	820.0305	-2.85E-01	0.00
103	828.1392	6.13E-02	0.00
104	835.7903	-1.16E+00	0.00
105	843.2402	-8.30E-02	0.00
106	847.065	8.88E-01	0.00
107	852.3784	-9.11E-01	0.00
108	871.2632	2.68E+00	0.01
109	880.3899	2.15E-01	0.00
110	882.5171	-9.43E-01	0.00
111	884.6808	8.97E-01	0.00
112	892.8862	-1.07E+00	0.00
113	893.9343	-8.99E+00	0.17
114	911.0012	-6.73E-01	0.00
115	911.2792	-3.38E-01	0.00
116	913.038	-3.93E-01	0.00
117	915.7858	2.41E-01	0.00
118	918.7109	-2.86E-03	0.00
119	930.0933	-2.26E-01	0.00

120	932.2049	5.07E-02	0.00
121	941.3954	-8.08E-02	0.00
122	945.3529	4.76E-02	0.00
123	949.4967	-2.53E-02	0.00
124	950.6005	-1.85E-02	0.00
125	952.0432	-7.69E-02	0.00
126	952.444	-8.76E-02	0.00
127	955.5594	-8.18E-02	0.00
128	958.9882	-2.59E-02	0.00
129	962.2329	4.46E-03	0.00
130	964.8031	5.82E-02	0.00
131	966.2659	-6.46E-02	0.00
132	972.428	-2.75E-01	0.00
133	973.219	9.45E-01	0.00
134	974.2346	5.97E-01	0.00
135	975.9536	5.70E-02	0.00
136	978.9079	-1.17E-02	0.00
137	979.8134	-4.50E-01	0.00
138	986.7484	1.37E-01	0.00
139	990.1476	9.34E-02	0.00
140	991.0828	-6.57E-02	0.00
141	994.5761	-1.68E-01	0.00
142	997.0875	7.72E-01	0.00
143	1002.698	2.46E-01	0.00
144	1012.416	4.06E-02	0.00
145	1019.009	1.43E-01	0.00
146	1019.308	-7.02E-02	0.00
147	1033.516	-4.04E+00	0.04
148	1035.232	2.26E+00	0.01
149	1041.387	9.26E-01	0.00
150	1053.06	3.83E-01	0.00
151	1064.36	-6.00E-02	0.00
152	1072.135	2.97E+00	0.02
153	1074.431	-3.43E-01	0.00
154	1075.862	2.02E-01	0.00
155	1079.949	3.45E-01	0.00
156	1090.658	-5.48E-03	0.00
157	1101.37	5.74E+00	0.08
158	1104.315	-3.68E+00	0.03
159	1115.719	-1.85E-01	0.00
160	1133.793	-1.98E+00	0.01
161	1137.92	7.37E+00	0.14
162	1145.194	5.83E+00	0.09
163	1150.112	-6.59E-03	0.00
164	1153.483	-2.12E+00	0.01
165	1154.317	-3.34E+00	0.03
166	1170.14	-7.73E-01	0.00
167	1181.362	-5.57E-01	0.00
168	1190.713	-4.61E-01	0.00
169	1192.001	2.92E+00	0.02
170	1194.447	3.77E-02	0.00



171	1195.289	-1.31E-01	0.00
172	1210.123	-2.15E-01	0.00
173	1245.172	-4.93E-01	0.00
174	1262.847	2.35E-01	0.00
175	1265.039	-1.31E+00	0.00
176	1272.592	7.24E-01	0.00
177	1296.138	-1.50E+00	0.01
178	1300.976	2.01E-01	0.00
179	1315.091	5.01E+00	0.08
180	1330.282	4.70E+00	0.07
181	1333.136	-2.39E-01	0.00
182	1339.126	7.40E-02	0.00
183	1341.133	9.92E-02	0.00
184	1344.288	1.76E-01	0.00
185	1346.354	-1.70E-01	0.00
186	1359.496	-5.43E+00	0.09
187	1383.466	-2.89E+00	0.03
188	1398.296	3.18E-01	0.00
189	1408.187	-2.71E-01	0.00
190	1430.469	-3.22E-01	0.00
191	1432.538	-3.63E+00	0.04
192	1457.915	-6.36E-01	0.00
193	1473.715	2.10E+00	0.01
194	1476.755	-2.30E-01	0.00
195	1488.329	-6.55E-01	0.00
196	1490.326	1.41E+00	0.01
197	1491.251	9.33E-01	0.00
198	1500.451	-5.84E-01	0.00
199	1510.514	-1.30E+00	0.01
200	1524.424	1.26E+00	0.01
201	1530.019	-3.51E-01	0.00
202	1533.782	1.07E-01	0.00
203	1562.269	-8.68E+00	0.27
204	1570.721	-8.96E-01	0.00
205	1582.132	2.74E+00	0.03
206	1614.295	-4.89E-02	0.00
207	1622.311	1.43E+00	0.01
208	1630.319	7.47E-01	0.00
209	1641.523	-5.55E+00	0.12
210	1643.432	-9.19E-02	0.00
211	1648.992	8.64E-01	0.00
212	1659.393	3.23E-01	0.00
213	1682.687	5.41E-02	0.00
214	1685.29	-7.48E-02	0.00
215	1699.026	-9.09E-02	0.00
216	2684.078	-1.24E-02	0.00
217	2686.37	-1.19E-02	0.00
218	2686.991	-8.03E-03	0.00
219	2690.321	3.43E-03	0.00
220	2696.207	-1.15E-02	0.00
221	2697.684	-1.49E-02	0.00

222	2706.981	7.75E-03	0.00
223	2722.104	1.02E-01	0.00
224	2739.454	-9.57E-03	0.00
225	2785.952	-3.06E-02	0.00
226	3196.604	3.25E-02	0.00
227	3205.474	3.15E-02	0.00
228	3207.586	1.16E+00	0.01
229	3211.46	4.44E-01	0.00
230	3216.724	1.96E-02	0.00
231	3221.432	-2.18E-01	0.00
232	3228.41	-8.79E-01	0.01
233	3229.673	-1.77E-02	0.00
234	3230.205	-2.12E-02	0.00
235	3232.069	9.92E-02	0.00
236	3234.663	-1.88E-02	0.00
237	3236.42	1.70E-02	0.00
238	3240.28	1.03E-02	0.00
239	3243.519	1.52E+00	0.02
240	3249.74	-1.19E-02	0.00
241	3252.881	2.50E-01	0.00
242	3258.916	-3.23E-02	0.00
243	3261.376	1.98E-02	0.00
244	3264.01	4.53E-01	0.00
245	3268.795	-3.86E-02	0.00
246	3270.167	-2.11E-01	0.00
247	3270.435	4.47E-03	0.00
248	3294.543	3.24E-02	0.00
249	3302.603	-1.62E-02	0.00

**Table S11.** Vibrational frequencies ( $\omega_i/\text{cm}^{-1}$ ) at the respective optimized  $S_0$  states, Shift vector  $K_i$  (a.u.) and Huang-Rhys factor  $S_i$  of complex **5**.

	$\omega_i/\text{cm}^{-1}$	$K_i$ (a.u.)	$S_i$
1	24.1717	4.37E+01	0.11
2	25.5456	2.21E+01	0.03
3	36.3079	6.20E+00	0.00
4	39.7951	-3.74E+01	0.13
5	45.1158	-1.79E+01	0.03
6	55.3301	-7.55E+00	0.01
7	60.9644	-1.98E+01	0.05
8	64.4509	-6.94E+00	0.01
9	87.7979	-1.01E+00	0.00
10	97.0771	-1.94E+00	0.00
11	104.6369	2.22E+01	0.12
12	114.032	-2.69E+01	0.19
13	126.4037	8.05E+00	0.02
14	132.6438	1.31E+01	0.05
15	133.21	-1.15E+01	0.04
16	145.0019	1.02E+01	0.03
17	150.7964	3.36E+00	0.00
18	163.9196	1.13E+01	0.05

19	176.0051	-2.91E+00	0.00
20	196.9196	-9.09E+00	0.04
21	203.2724	8.16E+00	0.03
22	209.5543	8.69E+00	0.04
23	220.4823	8.69E+00	0.04
24	240.6291	7.76E-01	0.00
25	243.8097	-1.92E+01	0.21
26	260.5489	4.20E+00	0.01
27	270.4587	2.98E-01	0.00
28	272.257	3.39E+00	0.01
29	280.4078	-1.56E+00	0.00
30	287.3718	8.36E+00	0.05
31	305.0504	-2.84E+00	0.01
32	314.9287	-5.66E-01	0.00
33	336.5123	-1.67E+00	0.00
34	339.4087	3.19E+00	0.01
35	365.1544	6.85E-01	0.00
36	369.4169	-1.81E+00	0.00
37	383.1457	-1.27E+00	0.00
38	388.5156	6.57E+00	0.04
39	416.0573	1.65E+00	0.00
40	430.7055	1.17E+00	0.00
41	454.6607	1.14E-01	0.00
42	467.2761	-4.75E-01	0.00
43	475.0396	-1.72E+00	0.00
44	481.4288	-4.51E-01	0.00
45	486.9692	-1.14E-01	0.00
46	498.8932	1.39E+00	0.00
47	510.6257	-7.79E-01	0.00
48	514.8688	5.10E-01	0.00
49	519.4222	5.16E+00	0.03
50	523.3776	6.79E-01	0.00
51	531.1475	4.62E+00	0.03
52	531.7615	2.42E+00	0.01
53	549.3389	3.23E-01	0.00
54	556.6053	9.01E+00	0.10
55	562.5324	6.60E+00	0.06
56	569.7436	-2.72E-01	0.00
57	581.0085	-8.45E+00	0.09
58	586.2553	2.12E+00	0.01
59	589.0272	-1.26E+00	0.00
60	590.4321	1.05E+00	0.00
61	598.8718	-3.25E-01	0.00
62	604.2955	5.61E-01	0.00
63	606.7061	-6.01E-01	0.00
64	625.7539	-1.90E-01	0.00
65	627.3455	2.53E-01	0.00
66	637.4675	5.76E-02	0.00
67	649.3402	-4.78E-01	0.00
68	655.0112	-1.22E-01	0.00
69	659.8452	-4.04E-01	0.00

70	668.7738	-1.22E-01	0.00
71	676.7746	1.20E+00	0.00
72	683.8873	3.36E-01	0.00
73	691.4833	1.13E-01	0.00
74	701.8937	-4.22E-01	0.00
75	706.0218	3.54E-01	0.00
76	709.2589	-4.25E-01	0.00
77	714.4272	2.37E-01	0.00
78	722.7173	1.03E-01	0.00
79	727.8064	3.52E-01	0.00
80	736.4692	1.30E+00	0.00
81	740.3436	-1.03E-01	0.00
82	741.3666	3.91E-01	0.00
83	743.7293	-4.99E-03	0.00
84	748.114	-1.32E-01	0.00
85	749.9988	-4.55E-01	0.00
86	753.2839	1.61E-01	0.00
87	754.4706	5.29E-01	0.00
88	758.2633	3.12E-01	0.00
89	761.0898	-8.50E-01	0.00
90	766.4132	1.25E-01	0.00
91	768.29	2.97E-01	0.00
92	769.0536	3.16E-01	0.00
93	772.3278	3.87E-01	0.00
94	776.4471	-3.13E-01	0.00
95	778.4159	7.84E-02	0.00
96	779.8175	1.86E-01	0.00
97	789.4306	4.44E-02	0.00
98	793.0571	1.73E-01	0.00
99	799.3215	2.44E-01	0.00
100	802.5356	-3.61E+00	0.02
101	804.6703	-9.08E-01	0.00
102	805.9273	4.16E-02	0.00
103	808.6594	1.10E-01	0.00
104	810.9151	3.09E-02	0.00
105	822.8625	-2.28E-01	0.00
106	826.5452	4.25E-01	0.00
107	849.2515	-2.02E-01	0.00
108	852.1017	-5.26E-02	0.00
109	872.5417	2.17E-02	0.00
110	874.1678	-3.92E-01	0.00
111	878.2751	5.77E-02	0.00
112	879.0645	2.36E-01	0.00
113	880.8313	-8.48E-02	0.00
114	889.9712	6.11E-01	0.00
115	892.3668	-3.44E-01	0.00
116	905.3856	-9.88E-02	0.00
117	912.1057	-1.31E-01	0.00
118	917.0702	-1.32E-01	0.00
119	919.0604	8.92E-02	0.00
120	930.5847	-1.52E-01	0.00

121	935.8901	-1.35E-02	0.00
122	941.1251	-8.42E-02	0.00
123	946.8457	3.03E-01	0.00
124	948.9969	-6.66E-02	0.00
125	950.8815	2.62E-01	0.00
126	953.3782	-1.08E-01	0.00
127	954.8517	3.63E-01	0.00
128	955.9963	-1.43E-01	0.00
129	956.9774	-2.04E-01	0.00
130	957.8158	-1.10E-01	0.00
131	959.3021	2.48E-02	0.00
132	962.5009	-1.78E-01	0.00
133	964.5142	9.42E-02	0.00
134	967.7856	1.65E-01	0.00
135	973.9029	1.12E+00	0.00
136	976.125	1.92E+00	0.01
137	979.5938	-1.10E-01	0.00
138	979.983	4.93E-02	0.00
139	984.0292	-6.65E-02	0.00
140	987.6921	-3.13E-01	0.00
141	995.1356	9.34E-02	0.00
142	1002.173	-9.81E-03	0.00
143	1003.634	1.46E-01	0.00
144	1007.375	-3.25E-02	0.00
145	1011.669	1.05E-02	0.00
146	1017.298	-5.62E-01	0.00
147	1020.148	1.37E-03	0.00
148	1036.014	-9.76E-02	0.00
149	1041.981	7.56E-02	0.00
150	1046.463	-1.77E+00	0.01
151	1051.731	-1.19E+00	0.00
152	1059.288	1.22E+00	0.00
153	1063.61	-2.90E+00	0.02
154	1065.948	1.02E+00	0.00
155	1068.968	-1.13E-02	0.00
156	1078.588	4.65E-01	0.00
157	1078.632	-1.28E+00	0.00
158	1091.784	-1.04E+00	0.00
159	1093.612	-8.82E-01	0.00
160	1102.76	-2.29E+00	0.01
161	1118.143	6.49E-02	0.00
162	1150.766	3.93E-02	0.00
163	1158.615	4.97E-01	0.00
164	1160.435	4.45E-01	0.00
165	1173.627	1.08E+00	0.00
166	1174.582	1.42E+00	0.01
167	1181.485	-2.86E+00	0.02
168	1192.419	-2.44E-02	0.00
169	1196.062	-3.48E-03	0.00
170	1198.667	1.83E-01	0.00
171	1202.226	-2.04E+00	0.01

172	1211.545	-2.64E+00	0.02
173	1236.629	2.60E-01	0.00
174	1245.064	-5.48E-02	0.00
175	1272.155	5.09E-02	0.00
176	1286.19	-3.01E-01	0.00
177	1291.519	-2.35E+00	0.02
178	1305.482	3.29E-01	0.00
179	1323.813	-3.59E-02	0.00
180	1335.868	2.93E-01	0.00
181	1340.687	-5.41E+00	0.09
182	1343.486	-1.63E+00	0.01
183	1345.034	-3.33E-01	0.00
184	1345.645	-1.97E-01	0.00
185	1358.408	5.13E-02	0.00
186	1377.648	6.40E+00	0.13
187	1390.286	9.49E-02	0.00
188	1403.25	4.71E+00	0.07
189	1414.264	-1.48E-01	0.00
190	1425.35	-8.45E+00	0.23
191	1452.175	4.83E-02	0.00
192	1463.811	-1.02E-01	0.00
193	1473.255	-2.15E-01	0.00
194	1486.032	1.88E-01	0.00
195	1490.164	-7.28E-01	0.00
196	1492.2	4.57E+00	0.07
197	1493.793	-1.91E-01	0.00
198	1509.926	-1.87E+00	0.01
199	1513.714	-2.56E+00	0.02
200	1523.082	8.37E+00	0.24
201	1533.479	7.38E-01	0.00
202	1535.215	1.56E+00	0.01
203	1538.578	6.20E+00	0.14
204	1560.16	1.77E+00	0.01
205	1560.754	6.09E-01	0.00
206	1607.052	-2.37E+00	0.02
207	1634.464	2.65E-01	0.00
208	1640.936	-5.99E+00	0.13
209	1650.096	1.71E-01	0.00
210	1651.216	-2.79E-01	0.00
211	1660.324	-3.21E+00	0.04
212	1665.58	-5.05E-01	0.00
213	1681.111	8.23E-02	0.00
214	1686.161	6.95E-02	0.00
215	1713.962	-3.75E-02	0.00
216	2679.689	2.37E-02	0.00
217	2684.602	-3.23E-03	0.00
218	2686.795	1.13E-02	0.00
219	2692.005	-1.64E-02	0.00
220	2697.107	-1.13E-02	0.00
221	2699.973	-1.73E-02	0.00
222	2708.649	2.31E-02	0.00

223	2719.817	-1.60E-02	0.00
224	2734.695	-1.37E-03	0.00
225	2776.048	-9.26E-02	0.00
226	3201.864	-1.61E-03	0.00
227	3208.489	2.57E-02	0.00
228	3209.03	1.48E-02	0.00
229	3209.993	5.99E-02	0.00
230	3214.335	2.83E-04	0.00
231	3214.668	-7.01E-04	0.00
232	3221.761	-1.56E-03	0.00
233	3222.895	-6.69E-02	0.00
234	3226.235	-4.72E-02	0.00
235	3228.939	1.92E-02	0.00
236	3231.706	2.89E-03	0.00
237	3234.545	-8.21E-03	0.00
238	3235.577	-1.72E-02	0.00
239	3238.198	-7.68E-03	0.00
240	3241.892	-2.43E-03	0.00
241	3242.462	5.08E-02	0.00
242	3243.569	6.61E-02	0.00
243	3244.746	1.97E-03	0.00
244	3249.994	2.74E-02	0.00
245	3258.569	-2.46E-01	0.00
246	3261.67	-3.07E-02	0.00
247	3268.183	4.48E-03	0.00
248	3281.122	-2.38E-02	0.00
249	3284.679	3.08E-01	0.00

**Table S12.** Vibrational frequencies ( $\omega_i/\text{cm}^{-1}$ ) at the respective optimized  $S_0$  states, Shift vector  $K_i$  (a.u.) and Huang-Rhys factor  $S_i$  of complex **5a**.

	$\omega_i/\text{cm}^{-1}$	$K_i$ (a.u.)	$S_i$
1	23.3028	-1.41E+02	1.05
2	26.524	-1.11E+02	0.75
3	34.6044	-7.49E+01	0.44
4	41.3289	-9.24E+01	0.81
5	44.921	7.63E-01	0.00
6	65.7973	1.80E+01	0.05
7	70.1682	5.09E+01	0.41
8	74.9498	-3.20E+01	0.18
9	84.3938	-2.84E+00	0.00
10	98.1448	2.01E+01	0.09
11	108.162	-3.04E+01	0.23
12	117.3233	-6.13E+00	0.01
13	125.6733	5.19E+00	0.01
14	127.2824	5.63E+00	0.01
15	141.595	-2.69E+00	0.00
16	158.0705	-4.41E+00	0.01
17	163.9889	-8.71E+00	0.03
18	166.6933	1.18E+01	0.05
19	188.6192	9.91E+00	0.04

20	195.8739	-3.23E+00	0.00
21	203.2633	7.77E+00	0.03
22	203.8616	-7.89E+00	0.03
23	211.2299	-6.41E+00	0.02
24	230.3147	4.99E+00	0.01
25	249.4449	1.85E+00	0.00
26	257.2579	-2.42E+01	0.34
27	270.4775	-2.08E+01	0.27
28	278.5929	-1.30E+00	0.00
29	284.9041	4.53E+00	0.01
30	296.5824	-3.98E+00	0.01
31	307.4684	4.27E+00	0.01
32	325.7797	2.48E-01	0.00
33	359.3554	9.66E-01	0.00
34	364.7619	1.19E+00	0.00
35	366.6435	3.95E-01	0.00
36	369.3127	8.33E-01	0.00
37	374.8501	1.77E-01	0.00
38	399.8327	-7.60E+00	0.05
39	423.2722	8.06E-01	0.00
40	446.576	5.19E+00	0.03
41	453.0101	1.79E+00	0.00
42	468.365	-1.15E+00	0.00
43	477.7654	-1.04E+01	0.12
44	484.0306	1.65E+00	0.00
45	490.6027	1.96E+00	0.00
46	498.8258	-1.42E+00	0.00
47	499.8943	-3.20E+00	0.01
48	513.8553	1.71E+00	0.00
49	516.9892	3.35E+00	0.01
50	522.1691	2.36E+00	0.01
51	525.9682	-9.69E+00	0.11
52	529.1067	6.80E+00	0.06
53	536.0668	-1.17E+01	0.17
54	548.069	5.04E-01	0.00
55	549.6806	3.18E-01	0.00
56	583.4827	2.00E+00	0.01
57	586.9486	2.83E+00	0.01
58	589.5235	1.09E+01	0.16
59	597.3054	-2.37E-01	0.00
60	601.1102	1.64E+00	0.00
61	602.7852	2.03E-01	0.00
62	603.1042	-7.08E-01	0.00
63	606.3869	9.70E-01	0.00
64	621.1445	2.23E+00	0.01
65	624.3509	-5.58E-01	0.00
66	634.4359	-8.62E-01	0.00
67	638.6424	3.73E+00	0.02
68	643.0945	5.99E-01	0.00
69	653.7793	4.23E-01	0.00
70	661.9977	4.72E+00	0.03

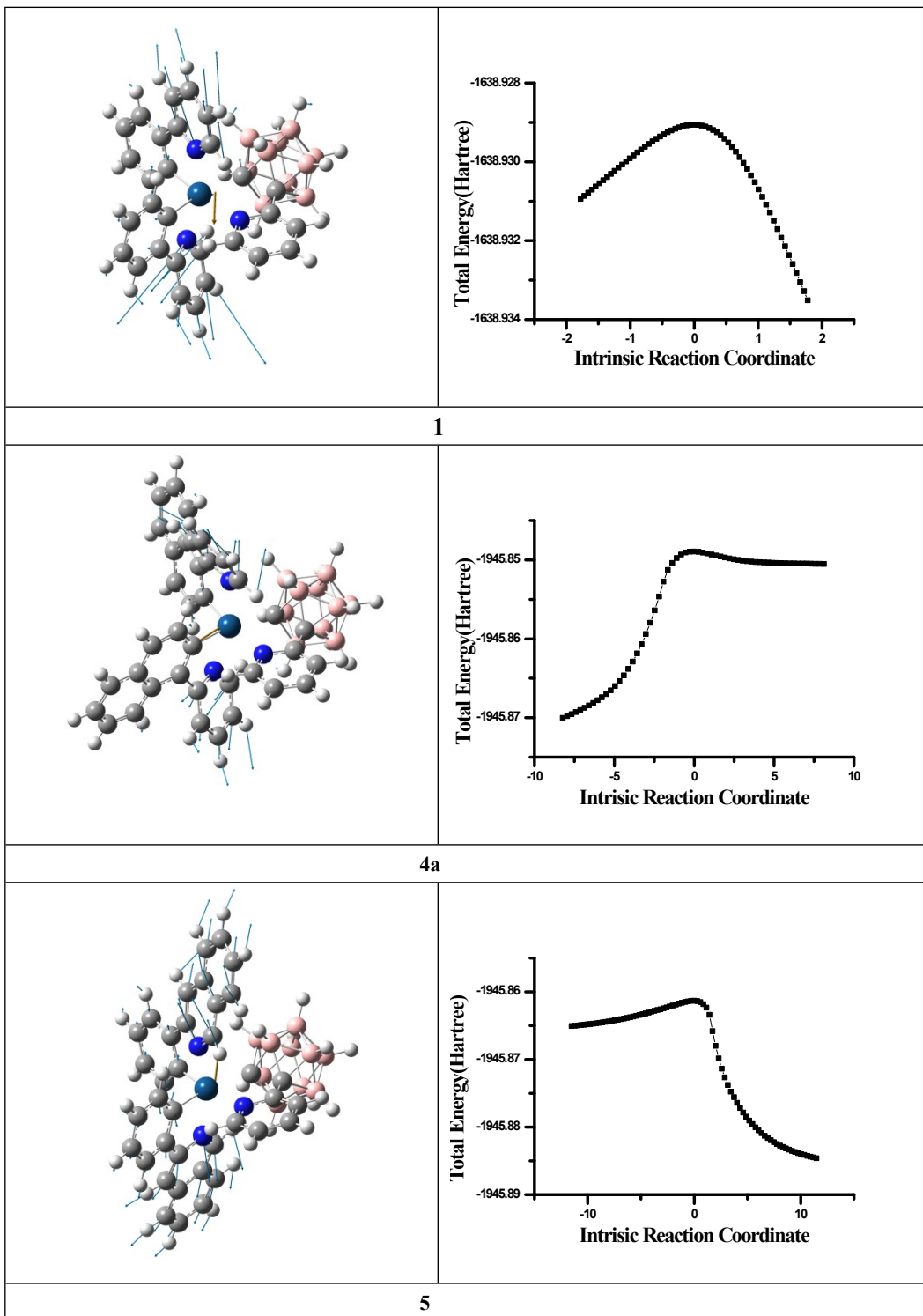


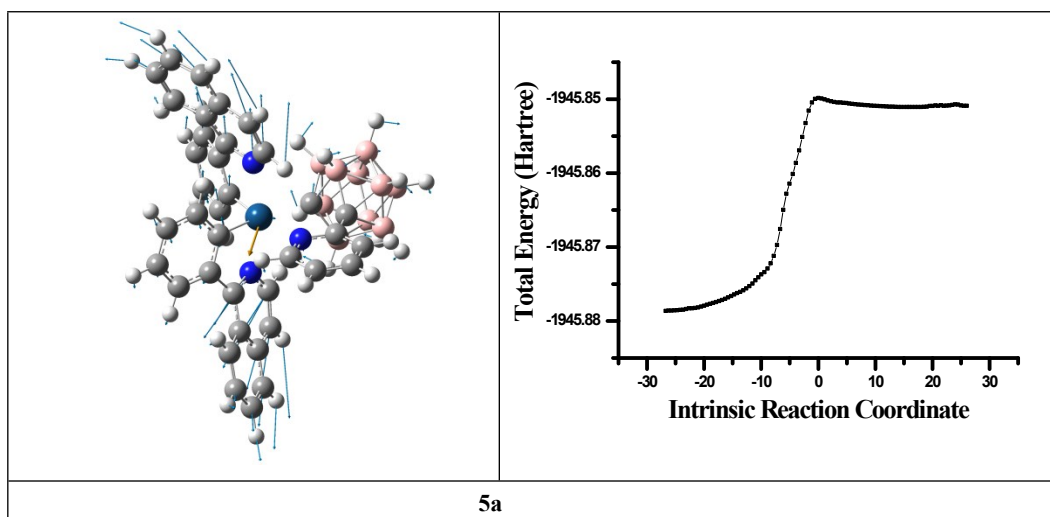
71	667.8647	-1.03E-01	0.00
72	682.7124	9.54E-01	0.00
73	699.3748	-1.58E-02	0.00
74	700.6798	-2.08E-01	0.00
75	704.8165	-4.00E-01	0.00
76	713.4902	3.04E+00	0.02
77	714.23	6.43E+00	0.07
78	727.1489	1.37E-01	0.00
79	730.3183	1.98E-01	0.00
80	739.3245	-6.89E+00	0.08
81	740.7618	-2.68E-01	0.00
82	745.6787	1.20E+00	0.00
83	748.2394	-1.25E-01	0.00
84	749.3014	-1.46E+00	0.00
85	755.3889	3.83E-01	0.00
86	758.5337	1.20E+00	0.00
87	762.993	3.51E-01	0.00
88	766.409	8.68E-02	0.00
89	767.8122	5.82E-01	0.00
90	769.6704	6.29E-01	0.00
91	772.701	-1.56E-01	0.00
92	775.4422	-6.37E-01	0.00
93	776.4738	-1.05E+00	0.00
94	781.7124	8.15E-01	0.00
95	783.7436	5.32E-02	0.00
96	788.8573	1.21E-01	0.00
97	789.717	2.66E+00	0.01
98	794.5552	-2.54E-01	0.00
99	795.6986	-6.08E-01	0.00
100	799.9439	3.88E-01	0.00
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104	830.7349	9.15E-01	0.00
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107	854.0555	8.63E-02	0.00
108	871.3235	2.30E+00	0.01
109	876.9153	3.02E-02	0.00
110	880.769	1.78E+00	0.01
111	884.4701	-1.63E+00	0.01
112	891.1848	-2.66E-01	0.00
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115	905.9914	6.65E-02	0.00
116	912.5829	-2.81E-01	0.00
117	917.0228	-1.78E-01	0.00
118	927.9039	-1.58E-02	0.00
119	938.1587	2.09E-01	0.00
120	938.6071	3.25E-01	0.00
121	939.8456	1.96E-01	0.00

122	940.2283	1.48E-01	0.00
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127	954.5276	-1.63E-01	0.00
128	958.3974	2.49E-01	0.00
129	959.0347	7.96E-02	0.00
130	962.6043	-4.61E-02	0.00
131	965.5326	-7.17E-01	0.00
132	968.4839	-4.50E-01	0.00
133	969.2695	1.61E-01	0.00
134	975.9384	1.26E+00	0.00
135	977.5501	3.81E-01	0.00
136	979.6227	1.57E-02	0.00
137	980.3581	3.84E-01	0.00
138	984.0867	2.92E-01	0.00
139	987.8843	-9.13E-01	0.00
140	991.7312	2.82E-02	0.00
141	991.9496	-1.17E+00	0.00
142	996.0014	6.39E-01	0.00
143	996.7712	-3.42E-01	0.00
144	1004.356	-3.02E-01	0.00
145	1015.647	-3.85E-02	0.00
146	1019.575	-2.90E-02	0.00
147	1021.116	-9.97E-01	0.00
148	1035.58	6.23E-01	0.00
149	1040.569	2.14E+00	0.01
150	1048.544	-6.48E+00	0.10
151	1063.649	-1.91E-01	0.00
152	1068.255	-2.52E-01	0.00
153	1071.192	5.26E-01	0.00
154	1074.005	2.59E-01	0.00
155	1078.772	1.84E-01	0.00
156	1088.341	-3.11E+00	0.02
157	1089.581	-1.36E+00	0.00
158	1093.141	6.13E+00	0.09
159	1113.567	2.55E-01	0.00
160	1128.077	-4.62E+00	0.06
161	1134.63	2.36E+00	0.01
162	1138.469	4.16E+00	0.05
163	1149.938	-1.28E-01	0.00
164	1158.704	-3.94E-02	0.00
165	1161.533	6.73E-01	0.00
166	1173.061	-4.01E-02	0.00
167	1189.283	7.27E-01	0.00
168	1191.632	-2.23E-01	0.00
169	1193.614	-3.24E+00	0.03
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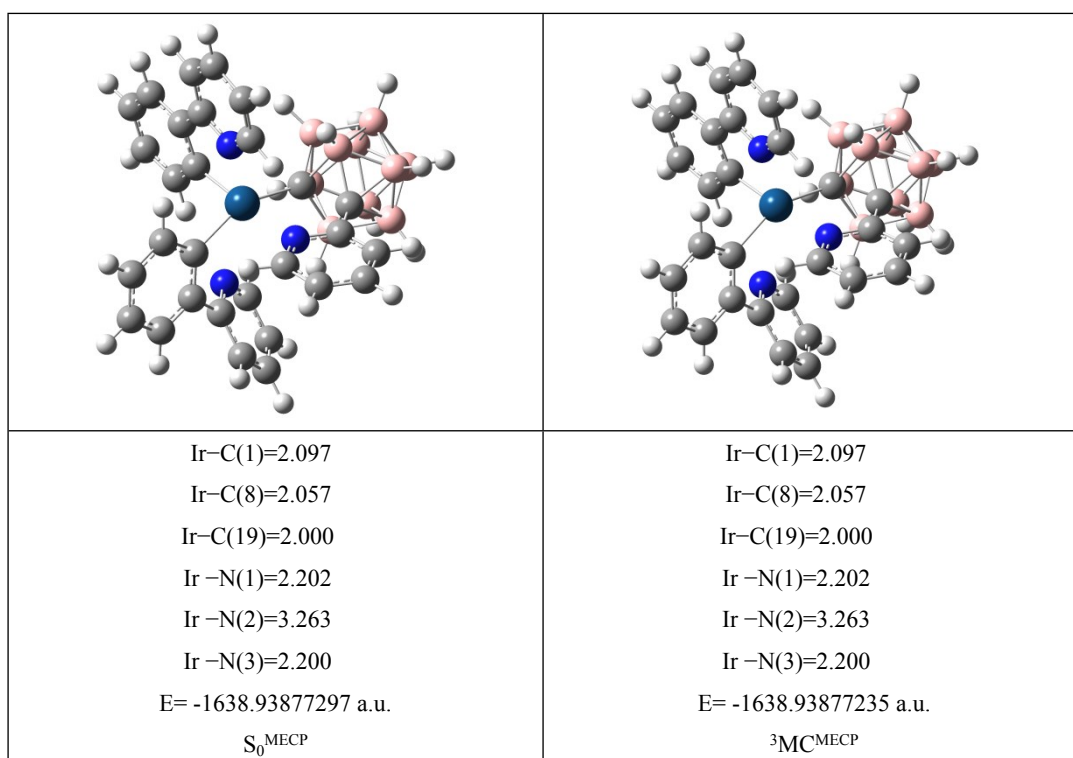
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176	1278.342	1.14E+00	0.00
177	1282.89	2.06E+00	0.01
178	1292.975	-4.86E-01	0.00
179	1318.965	3.61E+00	0.04
180	1328.606	9.79E+00	0.29
181	1332.181	-2.69E+00	0.02
182	1337.49	2.03E+00	0.01
183	1339.973	9.67E-02	0.00
184	1346.29	-1.01E-01	0.00
185	1362.212	-1.37E+00	0.01
186	1367.034	6.91E-01	0.00
187	1391.949	-1.11E-01	0.00
188	1406.971	3.51E+00	0.04
189	1422.189	4.83E-01	0.00
190	1426.145	3.62E+00	0.04
191	1447.392	3.32E-02	0.00
192	1455.115	-2.43E+00	0.02
193	1467.628	1.65E+00	0.01
194	1468.772	-4.63E+00	0.07
195	1474.685	2.89E-01	0.00
196	1484.545	2.90E+00	0.03
197	1489.741	1.73E-01	0.00
198	1491.371	2.54E-01	0.00
199	1509.468	-3.94E-02	0.00
200	1513.325	-8.35E-02	0.00
201	1526.669	-1.21E+00	0.01
202	1533.485	-2.32E-01	0.00
203	1563.105	-8.28E+00	0.24
204	1574.544	-3.73E-01	0.00
205	1583.357	5.44E-01	0.00
206	1612.097	-1.15E+00	0.00
207	1618.108	5.38E-02	0.00
208	1628.577	4.35E+00	0.07
209	1637.796	-7.52E-02	0.00
210	1642.932	-4.95E+00	0.09
211	1650.813	1.53E-01	0.00
212	1668.34	2.04E-01	0.00
213	1680.648	-1.04E-01	0.00
214	1686.421	3.44E-01	0.00
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217	2686.329	4.04E-02	0.00
218	2686.549	9.19E-02	0.00
219	2689.87	-2.11E-02	0.00
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221	2695.602	-2.68E-03	0.00
222	2704.804	-1.70E-01	0.00
223	2719.654	1.48E-01	0.00

224	2747.308	-1.57E-01	0.00
225	2773.411	9.98E-02	0.00
226	3204.243	-1.42E-01	0.00
227	3206.928	1.58E-03	0.00
228	3213.332	-4.83E-01	0.00
229	3215.003	-9.80E-04	0.00
230	3217.135	-8.08E-02	0.00
231	3221.592	-3.02E-02	0.00
232	3227.07	5.28E-03	0.00
233	3227.392	-1.16E-02	0.00
234	3228.417	1.35E-03	0.00
235	3233.494	-1.51E-01	0.00
236	3237.14	-1.01E-01	0.00
237	3239.231	1.25E-03	0.00
238	3240.917	-9.96E-03	0.00
239	3241.146	-6.10E-02	0.00
240	3241.747	-1.94E-02	0.00
241	3243.339	1.28E-01	0.00
242	3243.828	-1.93E-02	0.00
243	3248.178	3.56E-01	0.00
244	3248.903	1.96E-02	0.00
245	3256.734	1.12E-01	0.00
246	3267.299	-2.16E-01	0.00
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248	3284.925	1.03E-03	0.00
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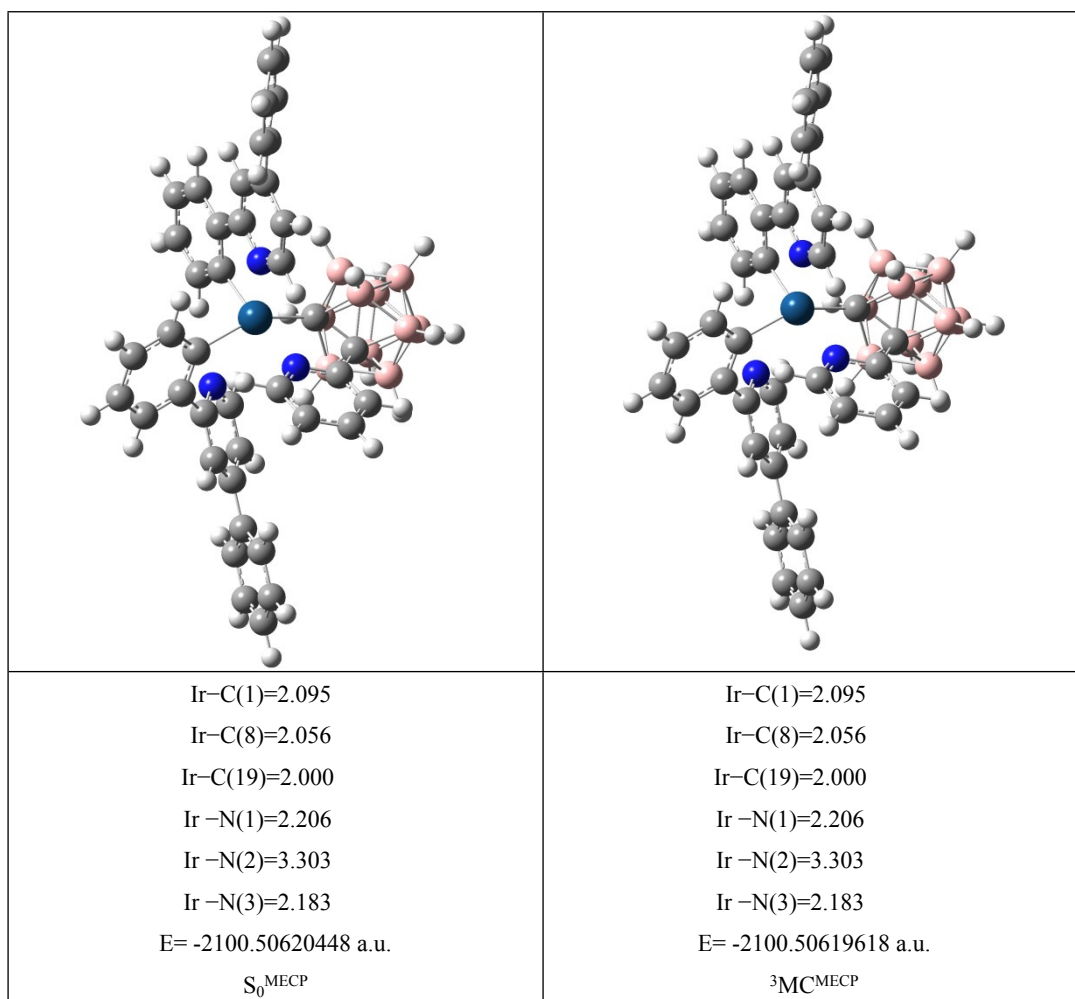




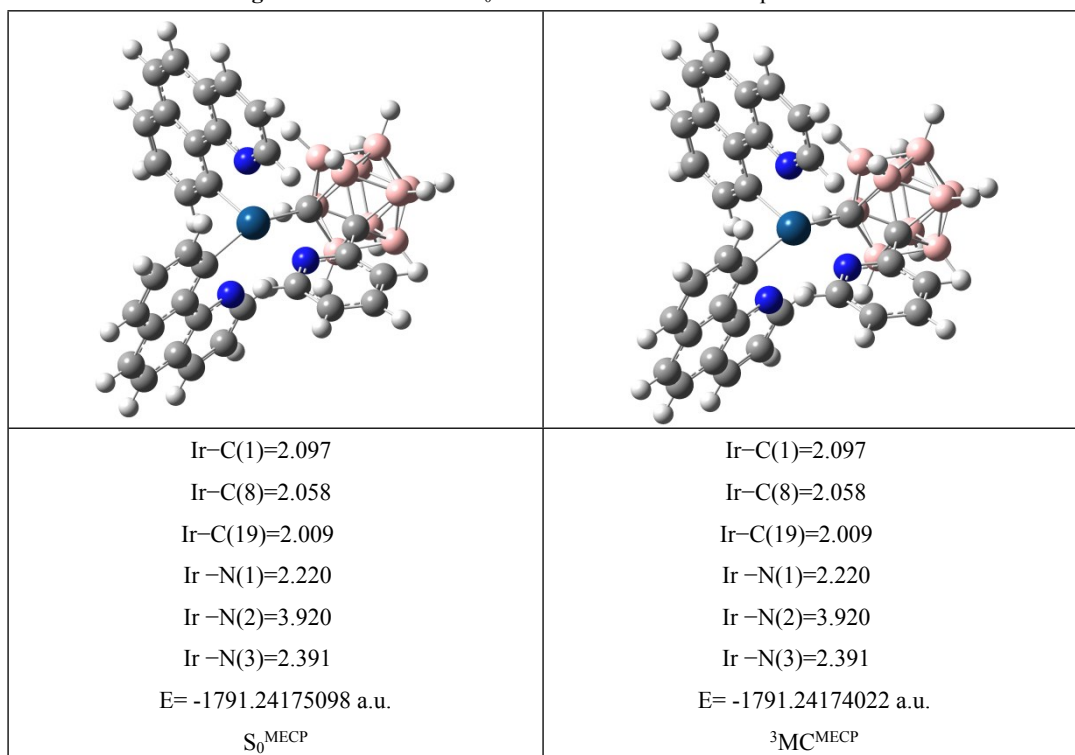
**Figure S1.** The vibration form and the curve of intrinsic reaction coordinate of  ${}^3\text{TS}[\text{}^3\text{ES}/\text{}^3\text{MC}]$  for complexes **1**, **4a**, **5**, **5a**.



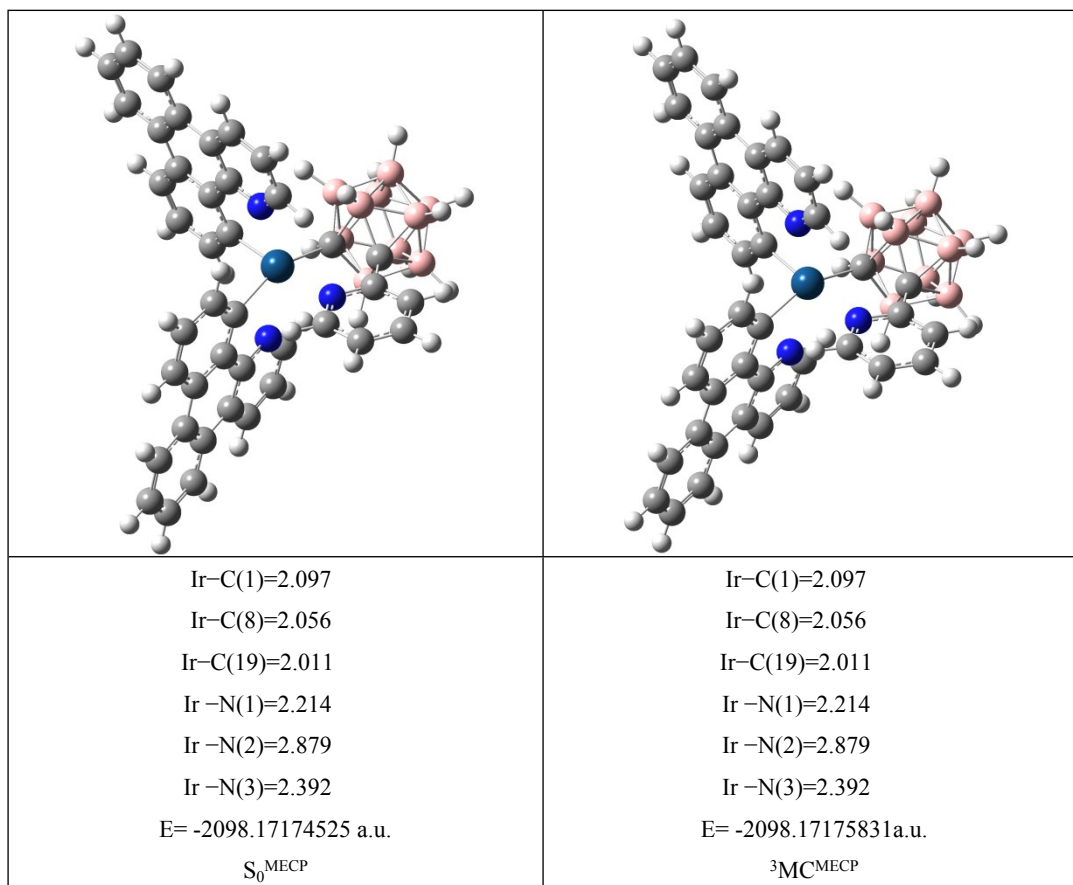
**Figure S2.** Structures of  $S_0$  and  ${}^3\text{MC}$  at MECP for complex **1**.



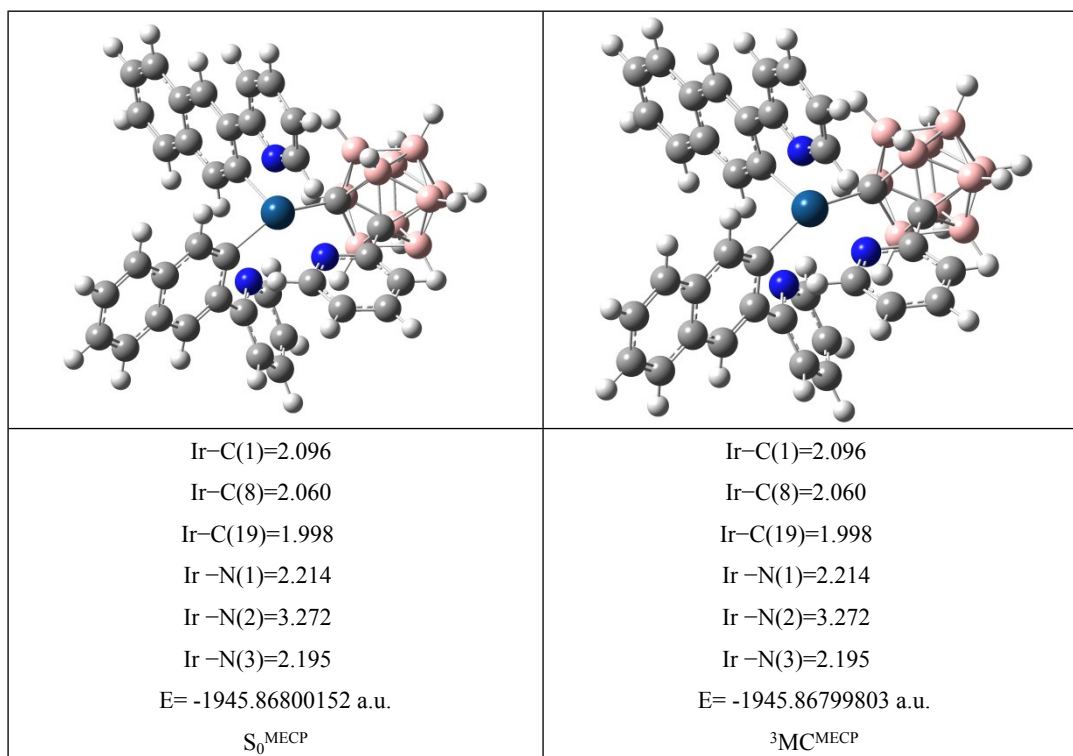
**Figure S3.** Structures of  $S_0$  and  ${}^3\text{MC}$  at MECP for complex 2.



**Figure S4.** Structures of  $S_0$  and  ${}^3\text{MC}$  at MECP for complex 3.

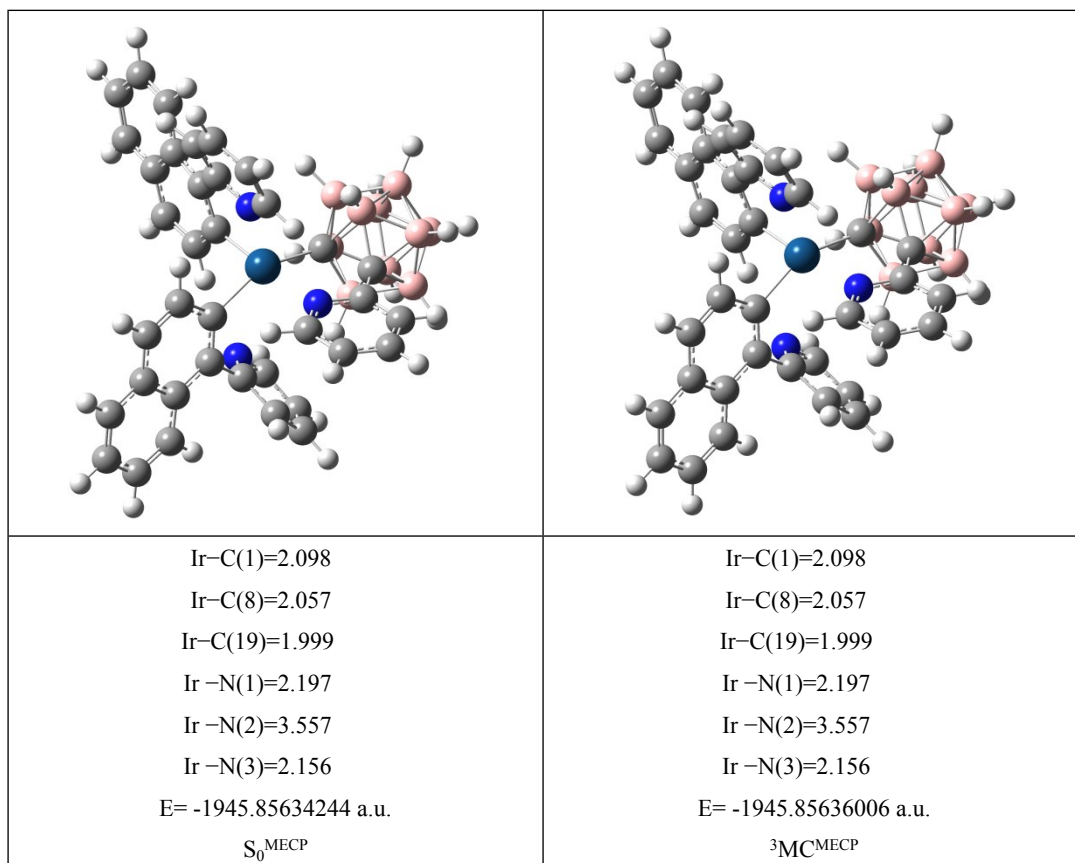


**Figure S5.** Structures of  $S_0$  and  ${}^3\text{MC}$  at MECP for complex **3a**.

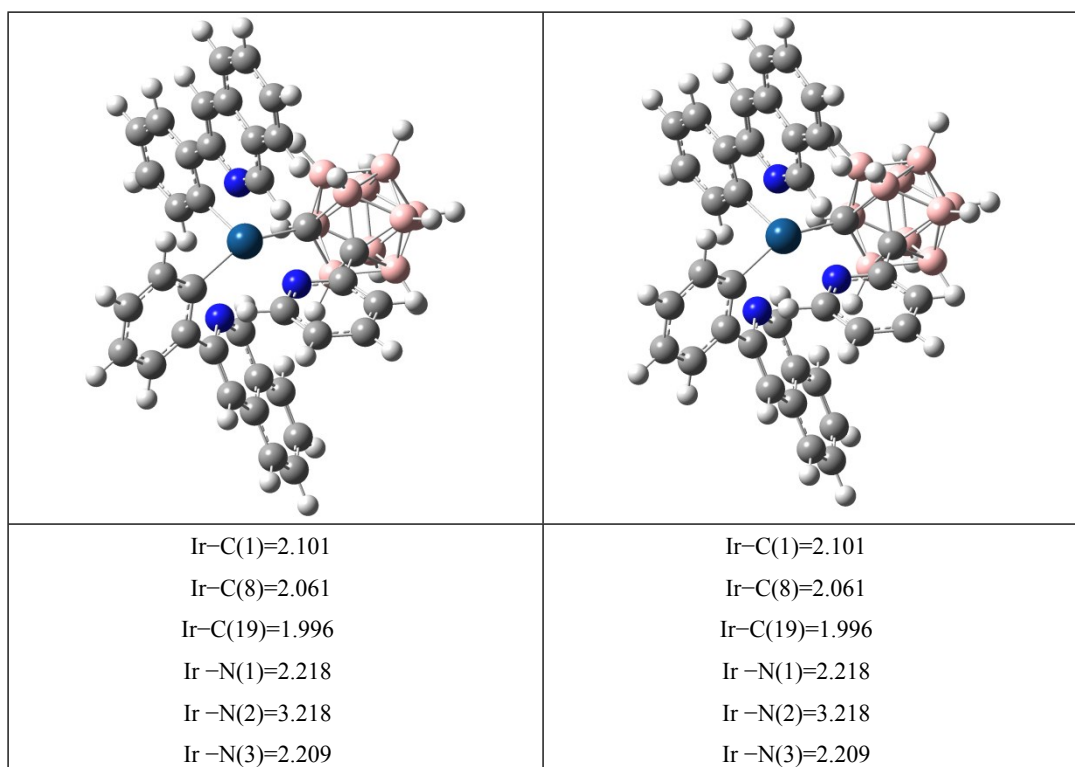


**Figure S6.** Structures of  $S_0$  and  ${}^3\text{MC}$  at MECP for complex **4**.



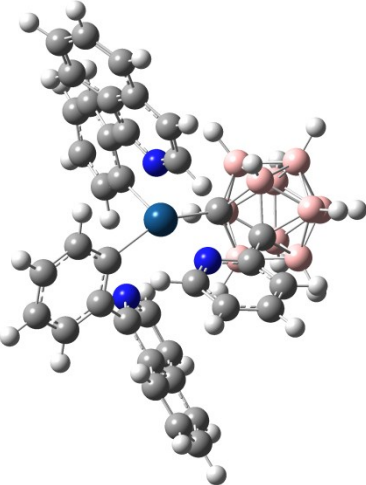
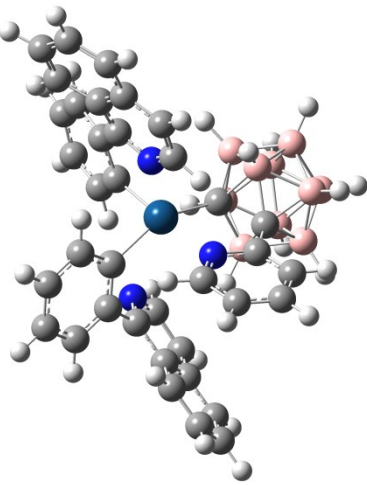


**Figure S7.** Structures of  $S_0$  and  ${}^3\text{MC}$  at MECP for complex **4a**.



$E = -1945.86691510 \text{ a.u.}$ $S_0^{\text{MECP}}$	$E = -1945.86690184 \text{ a.u.}$ ${}^3\text{MC}^{\text{MECP}}$
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**Figure S8.** Structures of  $S_0$  and  ${}^3\text{MC}$  at MECP for complex **5**.

	
$\text{Ir}-\text{C}(1)=2.104$ $\text{Ir}-\text{C}(8)=2.057$ $\text{Ir}-\text{C}(19)=1.998$ $\text{Ir}-\text{N}(1)=2.195$ $\text{Ir}-\text{N}(2)=3.448$ $\text{Ir}-\text{N}(3)=2.160$ $E = -1945.85701513 \text{ a.u.}$ $S_0^{\text{MECP}}$	$\text{Ir}-\text{C}(1)=2.104$ $\text{Ir}-\text{C}(8)=2.057$ $\text{Ir}-\text{C}(19)=1.998$ $\text{Ir}-\text{N}(1)=2.195$ $\text{Ir}-\text{N}(2)=3.448$ $\text{Ir}-\text{N}(3)=2.160$ $E = -1945.85701393 \text{ a.u.}$ ${}^3\text{MC}^{\text{MECP}}$

**Figure S9.** Structures of  $S_0$  and  ${}^3\text{MC}$  at MECP for complex **5a**.