

Supporting Information

Table S1- Properties of the ground state and the 11 lowest-lying $^1\pi\pi^*$ states of KC_{2,3} calculated at the TDDFT-B3LYP/6-31G** level. Labels indicate the serial number of each $^1\pi\pi^*$ state in the general excited state set. Column one reports the state energies referred to the ground state. The diagonal squares of the 12x12 matrix report the components of the state dipole moments. The squares of the upper triangle report the components of the transition dipole moments, while those of the lower triangle give the oscillator strengths.

E/eV	No	0	1	3	4	5	7	8	9	10	12	15	17	Pol.
0	0	1.007	12.368	-0.745	-6.320	-2.916	-0.327	-0.963	-1.726	1.504	0.678	-0.164	0.323	x
		2.468	-0.134	-0.682	0.434	-0.042	0.026	0.036	0.350	0.754	-0.078	0.675	0.251	y
2.993	1	3.916	-24.910	6.697	-4.786	6.403	-3.578	-1.892	-2.090	-0.177	1.523	0.289	x	
		1.736	4.939	-0.114	-0.087	-0.453	0.220	0.341	0.016	-0.010	-0.528	-0.019	-0.082	y
3.344	3	0.013	0.826	-6.363	-17.258	-10.606	-0.523	-4.530	6.632	-3.701	0.628	-0.731	-1.400	x
				3.753	-0.444	-0.486	-0.922	1.056	-0.108	-0.059	0.255	0.531	0.110	y
4.288	4	0.653	0.220	1.067	12.356	-6.983	-6.911	-0.743	-15.997	-9.769	-2.464	-0.135	0.094	x
					2.240	-0.428	0.060	0.383	-0.751	0.330	-0.792	0.354	0.848	y
4.560	5	0.147	0.137	0.520	0.051	-11.908	7.374	5.894	4.863	-13.258	0.310	1.500	-4.032	x
						3.417	0.378	-0.296	-0.610	0.265	-0.373	-0.209	0.377	y
4.747	7	0.002	0.242	0.006	0.083	0.039	12.376	3.660	-11.970	3.312	-11.147	6.801	-2.573	x
							3.272	0.753	-0.354	-0.360	-0.104	0.567	-0.216	y
5.323	8	0.019	0.114	0.162	0.003	0.094	0.030	-19.513	3.376	-3.525	-2.075	4.624	-15.956	x
								3.574	-0.087	0.130	0.125	-0.588	-0.214	y
5.512	9	0.065	0.034	0.362	1.190	0.081	0.416	0.008	14.865	9.018	0.557	-4.812	-2.802	x
									3.051	-0.121	-0.768	0.072	0.680	y
5.832	10	0.063	0.047	0.129	0.559	0.794	0.046	0.024	0.099	-19.259	-3.509	0.110	6.085	x
										2.620	0.374	-0.123	-0.211	y
5.987	12	0.011	0.004	0.005	0.043	0.036	0.584	0.011	0.002	0.007	17.646	3.382	6.117	x
											2.858	0.083	0.549	y
6.196	15	0.011	0.028	0.009	0.001	0.014	0.256	0.072	0.060	0.000	0.009	9.889	-4.159	x
												3.749	-0.078	y
6.372	17	0.010	0.001	0.023	0.006	0.113	0.041	1.016	0.027	0.076	0.055	0.012	-8.991	x
													2.617	y

Table S2- Properties of the ground state and the 10 lowest-lying ${}^1\pi\pi^*$ states of KC2 calculated at the TDDFT-B3LYP/6-31G** level. For other details see the legend of Table S1.

E/eV	No	0	2	3	4	6	7	8	11	12	19	20	Pol.
0 1A_1	0	2.637	-10.765	0.820	-6.004	-0.157	-0.081	0.900	-1.846	-0.941	-0.287	-0.157	x y
3.281 1B_2	2	1.442	5.292	-21.079	0.417	7.872	6.690	0.484	-0.187	-1.930	-0.514	-0.161	x y
3.652 1A_1	3	0.009	0.626	3.893	16.867	0.018	-1.703	-4.877	-5.911	-0.246	1.594	0.248	x y
4.794 1B_2	4	0.655	0.001	1.232	1.934	-12.399	3.913	-0.173	-0.975	14.257	1.479	1.669	x y
4.935 1A_1	6	0.000	0.389	0.000	0.082	3.544	-0.633	-5.565	13.427	-0.008	-4.636	0.108	x y
5.414 1A_1	7	0.000	0.362	0.019	0.036	0.001	3.085	15.368	9.107	-0.430	-10.916	-0.167	x y
5.637 1B_2	8	0.017	0.002	0.179	0.000	0.082	0.200	4.608	0.190	-4.133	0.062	-14.812	x y
6.153 1B_2	11	0.080	0.000	0.331	0.005	0.833	0.232	0.000	3.654	-13.702	1.224	4.524	x y
6.385 1A_1	12	0.021	0.044	0.001	1.281	0.000	0.001	0.048	0.165	2.750	-4.277	0.068	x y
6.727 1B_2	19	0.002	0.003	0.030	0.016	0.146	0.593	0.000	0.003	0.024	2.129	14.840	x y
6.842 1A_1	20	0.001	0.000	0.001	0.022	0.001	0.000	1.003	0.053	0.000	0.096	3.379	x y

Table S3- Properties of the ground state and the 14 lowest-lying $^1\pi\pi^*$ states of KC3 calculated at the TDDFT-B3LYP/6-31G** level. For other details see the legend of Table S1.

E/eV	No	0	1	3	4	5	7	8	9	10	11	12	16	17	18	19	Pol.
0 1A_1	0	2.322	13.610	0.620	8.227	0.336	-0.114	-1.726	2.900	0.649	-0.022	0.828	0.272	0.156	0.101	x y	
2.762 1B_2	1	1.940	4.711	30.058	0.373	6.512	-8.225	0.420	-0.179	-3.233	-0.577	0.663	1.453	0.818	-0.182	x y	
3.084 1A_1	3	0.004	1.105	-24.219	3.762	-0.404	-1.218	5.461	9.559	0.214	-0.797	-0.322	-0.673	-0.305	0.126	-2.745	x y
3.952 1B_2	4	1.015	0.001	1.931	2.042	-16.802	-3.748	-0.187	-1.038	21.335	0.855	0.824	0.549	-0.179	-4.789	0.767	x y
4.133 1A_1	5	0.002	0.221	0.001	0.194	3.288	0.497	-11.899	14.632	-0.082	-2.027	0.167	0.385	3.461	0.503	-2.921	x y
4.567 1A_1	7	0.000	0.461	0.008	0.033	0.004	2.604	-17.924	-16.691	13.197	0.370	0.050	-1.153	6.201	0.011	0.591	x y
4.627 1B_2	8	0.052	0.001	0.174	0.000	0.265	0.073	4.083	0.202	-7.934	0.069	-18.992	9.471	-0.120	0.153	0.367	x y
5.121 1B_2	9	0.163	0.000	0.706	0.005	0.802	0.585	0.000	2.737	-20.868	1.203	5.142	3.630	-0.078	14.525	0.635	x y
5.305 1A_1	10	0.019	0.101	0.000	2.335	0.000	0.000	0.162	0.304	2.687	-5.738	-0.033	-0.091	-2.588	0.021	17.833	x y
5.588 1B_2	11	0.009	0.004	0.006	0.005	0.023	0.674	0.000	0.003	0.035	2.199	22.461	3.323	0.010	0.382	-0.034	x y
5.621 1A_1	12	0.000	0.005	0.001	0.004	0.000	0.000	1.360	0.050	0.000	0.063	2.897	0.081	5.280	0.332	-12.717	x y
5.989 1A_1	16	0.016	0.026	0.004	0.002	0.001	0.007	0.463	0.043	0.000	0.002	0.000	3.218	-19.120	-0.300	1.112	x y
6.174 1B_2	17	0.002	0.000	0.001	0.000	0.093	0.234	0.000	0.000	0.022	0.000	0.058	0.256	3.981	11.923	0.472	x y
6.254 1A_1	18	0.001	0.009	0.000	0.199	0.002	0.000	0.000	0.906	0.000	0.000	0.000	0.000	0.043	3.036	-16.070	x y
6.259 1B_2	19	0.000	0.000	0.091	0.005	0.069	0.002	0.001	0.002	1.150	0.000	0.391	0.001	0.000	0.005	2.472	x y