Supporting Information

A Bis(acetyl)-Bridged Platinum(II) Coordination Polymer as Building Block for Diacetylplatinum(II) Complexes and Platina-β-diketones

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Energies and Cartesian coordinates of calculated molecules.

Complex ***10$_{calc}$***

File name: Br_dk_6311_C1.log

*E(*RB+HF-LYP) = –6001.6124116 au

E_{ZPC}: –6001.401528 au

	x	*y*	*z*
Pt	2.01229	0.00111	0.01451
C	3.38377	1.41806	0.00751
C	3.43956	–1.40273	0.08654
Pt	–2.01228	–0.00113	0.01476
C	–3.38381	–1.41830	0.00790
C	–3.43959	1.40246	0.08753
C	–3.10756	2.80241	0.54487
O	–4.61117	1.19044	–0.25226
O	–4.60194	–1.21302	–0.29007
C	–3.07197	–2.85730	0.29194
O	4.61050	–1.19126	–0.25526
C	3.10756	–2.80209	0.54590
C	3.07260	2.85683	0.29318
O	4.60171	1.21309	–0.29227
H	–4.75330	–0.15339	–0.39766

H	4.75301	0.15448	–0.40098
H	–4.03169	3.35385	0.72509
H	–2.52897	3.30417	–0.23572
H	–2.48303	2.78218	1.43850
H	–2.42223	–2.94724	1.16272
H	–2.51485	–3.26681	–0.55663
H	–3.99356	–3.42528	0.42795
H	2.48361	–2.78068	1.43990
H	4.03176	–3.35340	0.72620
H	2.52849	–3.30476	–0.23374
H	3.99442	3.42431	0.42977
H	2.42282	2.94616	1.16398
H	2.51575	3.26746	–0.55505
Br	0.03559	–1.72932	–0.14153
Br	–0.03557	1.72961	–0.14105

*Complex **10***$^{*}_{calc}$

File name: Br_dk_torsionfreeze.log

*E(*RB+HF-LYP) = –6001.5309079 au

	x	*y*	*z*
Pt	2.04601	–0.01117	0.01406
C	3.40846	1.37984	0.00715
C	3.48862	–1.44751	0.08731
Pt	–2.04599	0.01116	0.01432
C	–3.40851	–1.38005	0.00755
C	–3.48861	1.44724	0.08833
C	–3.14289	2.86531	0.55231
O	–4.62674	1.24856	–0.24136
O	–4.65502	–1.16253	–0.29763
C	–3.10405	–2.82576	0.29257
O	4.62626	–1.24947	–0.24433
C	3.14275	–2.86484	0.55333
C	3.10461	2.82538	0.29384

O	4.65463	1.16262	–0.29987
H	–5.15571	–1.99263	–0.35635
H	5.15524	1.99276	–0.35847
H	–4.07596	3.40046	0.72536
H	–2.56148	3.36282	–0.22829
H	–2.51743	2.85869	1.44700
H	–2.45517	–2.92279	1.16258
H	–2.54915	–3.23758	–0.55698
H	–4.01430	–3.42080	0.43482
H	2.51784	–2.85689	1.44839
H	4.07575	–3.40008	0.72651
H	2.56081	–3.36316	–0.22635
H	4.01514	3.41984	0.43669
H	2.45568	2.92184	1.16387
H	2.54997	3.23831	–0.55536
Br	0.02567	–1.75875	–0.14462
Br	–0.02561	1.75901	–0.14411

Complex ***11*** $_{calc}$

Datei: AcacDiketon_b3lyp_freq.log

*E(*RB+HF-LYP) = –771.9373193 au

E_{ZPC}: –771.721067 au

	x	*y*	*z*
Pt	0.41079	–0.00237	0.00432
C	1.79836	1.42286	–0.00927
C	1.77669	–1.40807	0.00199
C	1.42296	–2.85286	0.19202
O	3.02297	–1.19778	–0.14640
H	3.17854	–0.12354	–0.20227
C	1.38194	2.86417	0.15643
O	3.01470	1.20861	–0.15952
H	0.48441	–3.09573	–0.30247

H	1.25814	–3.01137	1.26454
H	2.24045	–3.49566	–0.13839
H	0.90098	2.99222	1.12984
H	0.62844	3.12562	–0.58791
H	2.25446	3.51387	0.07664
O	–1.16527	–1.48076	–0.02829
O	–1.13935	1.46378	–0.00817
C	–2.41748	–1.25553	–0.02705
C	–2.39702	1.25386	–0.00777
C	–3.03774	0.00551	–0.00977
H	–4.11893	0.01510	–0.01070
C	–3.28451	–2.49534	–0.05273
H	–4.34912	–2.26332	–0.02786
H	–3.06419	–3.06932	–0.95719
H	–3.03337	–3.12860	0.80237
C	–3.24106	2.50902	–0.01118
H	–3.01416	3.09260	–0.90782
H	–4.30945	2.29540	0.01508
H	–2.97465	3.12511	0.85178

*Complex **11***$^{*}_{calc}$

File name: acacDiketon_Torsionfixed.log

*E(*RB+HF-LYP) = –771.89281 au

	x	*y*	*z*
Pt	–0.40948	–0.01868	0.00390
C	–1.76513	–1.49132	–0.01182
C	–1.81628	1.35122	0.00307
C	–1.50188	2.80807	0.19538
O	–3.08464	1.10130	–0.14921
H	–3.60281	1.92315	–0.17446
C	–1.30120	–2.94325	0.15478
O	–2.95193	–1.31629	–0.15771
H	–0.56969	3.07519	–0.29958
H	–1.34186	2.96837	1.26855

H	–2.32146	3.46214	–0.12652
H	–0.81445	–3.07155	1.12634
H	–0.53912	–3.19511	–0.58539
H	–2.17024	–3.59427	0.07026
O	1.13451	1.51253	–0.02677
O	1.18383	–1.44369	–0.01015
C	2.38378	1.32357	–0.02558
C	2.44131	–1.19766	–0.00925
C	3.04623	0.06628	–0.00958
H	4.12733	0.08675	–0.01031
C	3.21714	2.58867	–0.04959
H	4.28890	2.39020	–0.02491
H	2.98009	3.15640	–0.95382
H	2.94718	3.21246	0.80681
C	3.31942	–2.42812	–0.01406
H	3.10932	–3.01699	–0.91131
H	4.38098	–2.18291	0.01269
H	3.07051	–3.05283	0.84791

Complex ***11*** $_{calc}$

File name: F3AcacDiketon_1.log

E(RB+HF-LYP) = –1367.5602031 au

EZPC: –1367.390424 au

	x	*y*	*z*
Pt	–1.17527	–0.01337	–0.00044
C	–2.57515	1.39799	0.00174
C	–2.52038	–1.43924	–0.00054
C	–2.11391	–2.88138	–0.02581
O	–3.77162	–1.24097	0.01683
H	–3.94870	–0.16591	0.02383
C	–2.14785	2.84373	–0.01670
O	–3.79243	1.16377	0.01907
H	–1.43449	–3.09030	0.80310

H	–1.54091	–3.07861	–0.93580
H	–2.99056	–3.52802	0.01866
H	–1.53124	3.03840	–0.89704
H	–1.51539	3.05579	0.84819
H	–3.02762	3.48776	–0.01508
O	0.45804	–1.47606	0.00158
O	0.40333	1.46303	–0.00078
C	1.68645	–1.21731	–0.01551
C	1.64251	1.24340	–0.01704
C	2.32847	0.02646	–0.03263
H	3.40580	0.04644	–0.05076
C	2.56525	–2.49072	0.00201
C	2.47209	2.54845	–0.00085
F	2.09695	3.35654	–1.00767
F	2.26988	3.20892	1.15556
F	3.79550	2.33303	–0.12096
F	3.87942	–2.22667	–0.12236
F	2.39070	–3.15507	1.16093
F	2.21758	–3.31549	–1.00131

*Complex **11***$^{*}_{calc}$

File name: F3AcacDiketon_Torsionfreeze2.log

*E(*RB+HF-LYP) = –1367.5178907 au

	x	*y*	*z*
Pt	–1.17149	0.00985	–0.00042
C	–2.57727	1.47279	0.00180
C	–2.53701	–1.39706	–0.00052
C	–2.15003	–2.84831	–0.02585
O	–3.81423	–1.17611	0.01724
H	–4.31852	–2.00679	0.02010
C	–2.13435	2.93756	–0.01681
O	–3.76142	1.25933	0.01865
H	–1.47381	–3.06515	0.80346

H	–1.58012	–3.05172	–0.93625
H	–3.01577	–3.51921	0.01743
H	–1.51493	3.14006	–0.89443
H	–1.49892	3.15675	0.84515
H	–3.02532	3.56277	–0.01466
O	0.44321	–1.47984	0.00162
O	0.42664	1.46171	–0.00075
C	1.66948	–1.24004	–0.01539
C	1.66772	1.22279	–0.01707
C	2.33293	0.00083	–0.03260
H	3.41045	0.00508	–0.05072
C	2.53023	–2.52679	0.00214
C	2.51589	2.51473	–0.00089
F	2.15398	3.32920	–1.00695
F	2.32441	3.17912	1.15492
F	3.83660	2.27844	–0.12115
F	3.84932	–2.28625	–0.12202
F	2.34663	–3.18978	1.16156
F	2.17061	–3.34741	–1.00193