SUPPORTING INFORMATION

An Alternative Structure for a Thermally Stable Cadmium Carbonyl Compound

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Received xxxx xx, 2020.

Table S1. Cartesian Coordinates for Geometry Optimized Molecules

$[Cd(CO)_3(C_6H_3Cl)]_4$			
atom	**x**	**y**	**z**
Cd	3.178538378	4.608968844	5.625229481
Cd	1.313439278	4.136041507	0.004273622
Cd	-3.599424237	1.336375233	1.931001009
Cd	-1.679115933	1.736046	7.550255278
Cl	1.317722107	4.989800617	3.070531544
Cl	-0.462434598	1.942862278	1.489336675
Cl	-2.643861785	2.695301481	4.650482657
Cl	1.114776663	2.161665487	6.07218042
O	5.248009691	1.426581904	6.822332441
O	1.910796319	8.402609912	5.071829765
O	6.180843914	6.555114641	7.309786074
O	1.04399667	8.100481374	0.457666374
O	2.815818499	0.573761938	-1.021709898
O	2.626310636	5.180882773	-3.607854707
O	-1.824747919	-2.112184785	0.917518961
O	-6.196086866	4.23740758	2.780076222
O	-6.718685822	-0.333306206	0.121831951
O	-4.581621245	4.458389247	7.956438215
O	0.960245293	-1.153944264	8.363642446
O	-3.015631498	0.585900148	11.11125363
C	4.925483327	2.47985472	6.550780243
C	2.502344243	7.482129805	5.373182856
C	5.323059752	5.971511959	6.851611545

C	1.040569803	7.031240173	0.077444038
C	2.488328883	1.656849889	-1.110306015
C	2.259212434	4.967333718	-2.556116647
C	-2.591529657	-1.276517101	0.962950694
C	-5.680165307	3.294450856	2.416842648
C	-5.858339748	0.186050839	0.64783578
C	-3.869796251	3.614239234	8.218986488
C	0.075625995	-0.446040832	8.303740003
C	-2.601456265	0.865348263	10.09299766
C	3.97217906	4.483853852	3.558999651
C	5.270959635	4.184788856	3.108492605
H	6.088025764	4.108748881	3.825467408
C	5.546193636	3.967017023	1.754780114
H	6.562537201	3.743050203	1.436387686
C	4.512881595	4.006885286	0.813294575
H	4.74878108	3.791661091	-0.228721073
C	3.187317312	4.299991092	1.183491974
C	3.016367499	4.549067469	2.545111337
C	-0.766675693	3.677783614	-0.611552174
C	-1.55464738	4.265972674	-1.617551634
H	-1.102615129	4.966871227	-2.318843022
C	-2.918775238	3.983485842	-1.740488981
H	-3.499865196	4.445398845	-2.536426273
C	-3.543788771	3.132860206	-0.82325685
H	-4.61684577	2.96549096	-0.915849766
C	-2.825574829	2.504693737	0.210761805
C	-1.460543164	2.79779338	0.221627995
C	-3.80921198	0.329615642	3.898655936

C	-4.286970376	-0.958852619	4.201048076
H	-4.764426075	-1.555459236	3.42377424
C	-4.15653394	-1.508706468	5.480354051
H	-4.545464716	-2.504026736	5.686577915
C	-3.499236938	-0.79440474	6.4867536
H	-3.373125873	-1.264237251	7.461749506
C	-2.991157647	0.498582232	6.263599101
C	-3.21581871	0.988341353	4.976255223
C	-0.234401543	3.292253084	8.179972816
C	-0.364376353	4.281311267	9.172418547
H	-1.206650228	4.246399602	9.863036229
C	0.554171312	5.329063593	9.289930253
H	0.428904374	6.077326221	10.07029843
C	1.61445869	5.434676454	8.384449403
H	2.290901898	6.284834896	8.470852515
C	1.812373729	4.486474293	7.363359724
C	0.87666622	3.45226791	7.351978184

$[Cd(C_6H_3Cl)]_4$

atom	**x**	**y**	**z**
Cd	3.057229929	4.630036566	5.58438379
Cd	1.316959394	3.983152783	0.107363375
Cd	-3.469381849	1.292592954	1.957090516
Cd	-1.704667509	1.895200299	7.429538106
Cl	1.256159376	4.963637521	3.055371391
Cl	-0.423346525	1.791630413	1.485423485
Cl	-2.638387894	2.740649081	4.586942818

Cl	1.006061919	2.304407776	5.945337476
C	3.935841584	4.649849359	3.56793909
C	5.257476707	4.449327914	3.133917981
H	6.070464743	4.447396735	3.856925509
C	5.555961802	4.237918753	1.784720391
H	6.588687584	4.094554129	1.475324379
C	4.531034367	4.172601322	0.836485021
H	4.787482523	3.958732655	-0.198988931
C	3.187095952	4.365108064	1.19875501
C	2.979326831	4.631251416	2.552482603
C	-0.697381132	3.513075886	-0.636700631
C	-1.466187221	4.100728483	-1.656110588
H	-1.002456838	4.796327509	-2.352168344
C	-2.829154797	3.819705768	-1.791058284
H	-3.399771316	4.280537427	-2.594095677
C	-3.470974238	2.978838912	-0.876948926
H	-4.542088251	2.816080353	-0.977201059
C	-2.763890928	2.356149338	0.165900008
C	-1.397888425	2.639085382	0.195700092
C	-3.867005311	0.377492356	3.917886819
C	-4.401779689	-0.874973397	4.265922013
H	-4.881977805	-1.4892981	3.507357943
C	-4.320774635	-1.360361956	5.574708847
H	-4.751577033	-2.328327436	5.820293513
C	-3.656718934	-0.625768388	6.561760504
H	-3.566831327	-1.050225891	7.559549285
C	-3.098814979	0.634038311	6.284899806
C	-3.276479609	1.074105335	4.972878457

C	-0.177144929	3.262118294	8.229842786
C	-0.19683713	4.127190721	9.33726646
H	-0.995879818	4.049162668	10.07156343
C	0.788023527	5.103212559	9.515695518
H	0.753972334	5.753206463	10.38705627
C	1.795428082	5.272510399	8.561491072
H	2.521144686	6.070987699	8.701449196
C	1.877240032	4.443019585	7.430168411
C	0.894059904	3.455741137	7.357074246