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The first triple-decker complex with the $PtMe_3$ fragment: $CpCo(\mu\text{-}1,3\text{-}C_3B_2Me_5)PtMe_3$

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Cartesian coordinates and energies for structures optimized at PBE/L2

2 E = –20494.71896351 a.u.

78	-1.48499315	0.14803701	-0.00000965
27	1.99381579	-0.18736620	0.00000266
6	0.31586911	-1.36305594	-0.00000470
6	0.54472770	1.02315129	0.73537405
6	0.54473258	1.02315065	-0.73537906
6	3.76036797	0.58748242	-0.71550147
1	3.84116784	1.46368071	-1.35224568
5	0.35830254	-0.47080823	-1.30007636
6	0.27461313	-2.86988310	-0.00000439
1	0.75067986	-3.30595100	0.89186367
1	0.75068934	-3.30595031	-0.89186824
1	-0.77101895	-3.21895151	-0.00001015
6	-2.84655394	-0.53683760	1.40366777
1	-3.88884693	-0.37791663	1.10076920
1	-2.66117493	-0.01432443	2.35234090
1	-2.66603919	-1.61299489	1.53605881
6	0.75248717	2.26418226	-1.55934382
1	1.55044758	2.90584550	-1.15656087
1	-0.16585867	2.87249645	-1.58104423
1	1.00408625	2.01545977	-2.59877511
6	0.75248276	2.26418192	1.55933837
1	1.55043957	2.90584030	1.15654013
1	1.00407083	2.01547626	2.59877588
1	-0.16585930	2.87250457	1.58101895
6	-2.65042970	1.85312379	-0.00001178
1	-3.72746913	1.64449878	-0.00000680
1	-2.40103650	2.43662450	-0.89866509
1	-2.40103235	2.43662167	0.89864238
6	0.38751763	-0.91250654	-2.82185463
1	0.86377373	-1.89628356	-2.95713736
1	0.92540179	-0.20035277	-3.46691861
1	-0.62838623	-1.00410154	-3.23792903
6	-2.84658552	-0.53686769	-1.40364535
1	-3.88886812	-0.37794383	-1.10071835
1	-2.66605888	-1.61302841	-1.53599770
1	-2.66120611	-0.01440541	-2.35234623
6	0.38751299	-0.91253260	2.82183905
1	0.86376971	-1.89631294	2.95709308
1	-0.62838893	-1.00414002	3.23791506
1	0.92539812	-0.20039294	3.46691794
6	3.58616650	-0.76086327	-1.16221667
1	3.51718105	-1.09148849	-2.19376440

6	3.76036067	0.58747644	0.71552799
1	3.84115038	1.46367067	1.35227894
6	3.47141200	-1.59031825	0.00000218
1	3.28475871	-2.66012681	-0.00000360
5	0.35829032	-0.47080551	1.30006991
6	3.58615401	-0.76087294	1.16222954
1	3.51715792	-1.09150963	2.19377287

CpCo(μ-1,3-$C_3B_2Me_5$)RuCp E = –6675.07299918 a.u.

44	-1.52267001	-0.05001725	-0.00000019
27	1.81519836	0.05671758	-0.00000070
6	0.26476797	2.82706751	0.00000035
1	-0.75512004	3.24073817	-0.00000013
1	0.77120708	3.22851378	-0.89177524
6	-3.30540648	-1.08753518	0.71706391
6	-3.35081817	1.11859305	0.00000092
6	0.27576561	-1.06783791	0.73423755
6	0.21079719	1.31875864	-0.00000016
6	-3.33715351	0.27775569	1.16379181
6	0.38795839	-2.32925980	1.54982126
1	1.25323145	-2.94181584	1.25195019
1	-0.50931468	-2.95257895	1.41790492
1	0.48173508	-2.10482688	2.62053475
5	0.22376121	0.43474378	1.31642283
6	0.32265025	0.87739766	2.83753671
1	0.84314772	1.84114523	2.95820739
1	0.85366110	0.14372591	3.46492575
1	-0.67571803	1.00661730	3.28372450
1	0.77120739	3.22851437	0.89177547
6	-3.30540703	-1.08753459	-0.71706359
6	0.27576595	-1.06783730	-0.73424058
6	-3.33715439	0.27775669	-1.16379056
6	0.38795851	-2.32925967	-1.54982376
1	1.25322951	-2.94181281	-1.25194068
1	-0.50930344	-2.95259358	-1.41790162
1	0.48174483	-2.10484506	-2.62054025
5	0.22376135	0.43474491	-1.31642419
6	0.32265025	0.87740113	-2.83753731
1	0.84314614	1.84114959	-2.95820757
1	0.85366021	0.14372995	-3.46492779
1	-0.67571858	1.00662144	-3.28372345
1	-3.37240789	2.20494828	0.00000101
1	-3.35359108	0.61402510	-2.19627751
1	-3.29025558	-1.96676768	-1.35518735
1	-3.29025443	-1.96676870	1.35518699
1	-3.35358919	0.61402267	2.19627928
6	3.53082929	-0.83019155	0.71584329
1	3.55331707	-1.70975816	1.35259252
6	3.53082966	-0.83019089	-0.71584497
1	3.55331765	-1.70975677	-1.35259510
6	3.43829051	0.52478800	1.16228873
1	3.38413728	0.85838317	2.19369007
6	3.43829090	0.52478903	-1.16228890
1	3.38413781	0.85838486	-2.19368998
6	3.37252734	1.36022794	0.00000038
1	3.24700287	2.43883976	0.00000099

Cp*$PtMe_3$ E = –18934.31171601 a.u.

78	-0.56945740	0.01175291	-0.00000472
6	1.42152867	1.19973938	-0.00000835
6	1.38211854	-1.01939263	-0.72744375

6	1.38211457	-1.01939059	0.72744911
6	1.41890030	0.34340817	1.16517893
6	1.57047435	2.68983340	-0.00000884
1	2.63120303	2.99183772	-0.00000757
1	1.10359460	3.14196666	0.88557950
1	1.10360024	3.14197026	-0.88559830
6	-1.84488263	0.86268219	-1.40076486
1	-2.90117686	0.69479008	-1.15597164
1	-1.63655629	0.42132041	-2.38611782
1	-1.66131352	1.94631034	-1.44113362
6	1.44943500	-2.24417274	1.58520738
1	2.47371761	-2.65004018	1.62058590
1	0.79704117	-3.04191010	1.20262796
1	1.14356253	-2.03392398	2.61806563
6	1.44945099	-2.24417092	-1.58520941
1	2.47373556	-2.65003500	-1.62058050
1	1.14359311	-2.03391214	-2.61806981
1	0.79705485	-3.04191254	-1.20264376
6	-1.88589156	-1.59695647	-0.00001257
1	-2.93533021	-1.27599252	-0.00000383
1	-1.70591152	-2.20783668	0.89701568
1	-1.70591749	-2.20782873	-0.89704724
6	1.49928582	0.81774901	2.58220698
1	2.54248043	1.03391990	2.86317697
1	1.11726007	0.06644525	3.28504155
1	0.92100256	1.73914329	2.73432629
6	-1.84487066	0.86264246	1.40077328
1	-2.90117221	0.69462715	1.15603375
1	-1.66151410	1.94631219	1.44115960
1	-1.63643660	0.42142112	2.38617782
6	1.49930234	0.81773596	-2.58221786
1	2.54249986	1.03390820	-2.86317706
1	0.92102081	1.73913065	-2.73434146
1	1.11728495	0.06643137	-3.28505500
6	1.41890531	0.34340068	-1.16518835

Cp*RuCp E = –5114.68791519 a.u.

44	-0.00001072	-0.00000145	0.43794624
6	-0.99451710	-0.72256033	-1.36096980
6	0.37986796	-1.16911995	-1.36089026
6	-0.99451773	0.72255575	-1.36096978
6	-2.20369394	-1.60110481	-1.46592959
1	-2.46474202	-1.79084522	-2.52083218
1	-3.07881691	-1.14183794	-0.98755578
1	-2.03733364	-2.57527162	-0.98746188
6	0.84176585	-2.59062553	-1.46552921
1	0.94153094	-2.89784413	-2.52034097
1	1.81967614	-2.73329388	-0.98704216
6	-2.20369409	1.60109923	-1.46592921
1	-2.46474298	1.79084817	-2.52083019
1	-2.03733207	2.57526742	-0.98746338
1	-3.07882057	1.14184146	-0.98755336
6	0.37707421	-1.16071731	2.26856868
1	0.71267659	-2.19363967	2.28328861
6	-0.98742240	-0.71735881	2.26852663
1	-1.86608304	-1.35573195	2.28319986
6	-0.98742299	0.71736130	2.26852535
1	-1.86608429	1.35573351	2.28319734
6	1.22938503	-0.00000118	-1.36124877
6	0.37986704	1.16911710	-1.36088961
6	2.72397265	-0.00000211	-1.46642522
1	3.04655546	-0.00000230	-2.52136336

1	3.16208294	0.88590604	-0.98804891
1	3.16208177	-0.88591069	-0.98804876
1	0.13457278	-3.28086588	-0.98693084
6	0.84176424	2.59062065	-1.46552831
1	0.94153122	2.89785387	-2.52033555
1	0.13457727	3.28086557	-0.98692550
1	1.81967114	2.73329616	-0.98703498
6	1.22037888	0.00000265	2.26859619
1	2.30645313	0.00000103	2.28334439
6	0.37707293	1.16072142	2.26856578
1	0.71267634	2.19364345	2.28328450