

From Two-Electron via Four-Electron to Six-Electron Donor Carbonyl Groups in Trinuclear Derivatives of the Oxophilic Metal Niobium

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Supporting Information

Tables S1 to S26. Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_n$ ($n = 9, 8, 7, 6$).

Tables S27 to S39. Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km/mol) of $\text{Cp}_3\text{Nb}_3(\text{CO})_n$ ($n = 9, 8, 7, 6$)

Table S1 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_9$ 9-1 C_3

	MPW1PW91/SDD			MPW1PW91/LANL2DZ		
Nb	0.000000	1.940504	-0.012369	0.000000	1.939229	-0.010997
Nb	1.680526	-0.970252	-0.012369	1.679421	-0.969614	-0.010997
Nb	-1.680526	-0.970252	-0.012369	-1.679421	-0.969614	-0.010997
C	1.530480	-0.547520	2.052424	1.530538	-0.543538	2.056940
O	1.672147	-0.445197	3.194148	1.678574	-0.437133	3.197259
C	0.543868	-1.488697	-1.700551	0.547976	-1.490795	-1.704293
O	0.301518	-1.920939	-2.760069	0.305256	-1.919920	-2.763906
C	-1.239406	-1.051675	2.052424	-1.235987	-1.053716	2.056940
O	-1.221625	-1.225523	3.194148	-1.217855	-1.235121	3.197259
C	-1.561184	0.273345	-1.700551	-1.565054	0.270836	-1.704293
O	-1.814341	0.699347	-2.760069	-1.815327	0.695600	-2.763906
C	1.017316	1.215352	-1.700551	1.017078	1.219959	-1.704293
O	1.512823	1.221592	-2.760069	1.510071	1.224319	-2.763906
C	-0.291074	1.599194	2.052424	-0.294551	1.597254	2.056940
O	-0.450522	1.670720	3.194148	-0.460719	1.672254	3.197259
C	1.913075	2.347862	0.617965	1.914562	2.348455	0.620893
O	2.957864	2.706731	0.982853	2.958512	2.707052	0.986923
C	1.076771	-2.830703	0.617965	1.076541	-2.832287	0.620893
O	0.865166	-3.914951	0.982853	0.865120	-3.915672	0.986923
C	-2.989846	0.482841	0.617965	-2.991103	0.483831	0.620893
O	-3.823029	1.208220	0.982853	-3.823631	1.208621	0.986923
C	0.188955	4.131034	-0.883927	0.179875	4.135363	-0.889092
C	-0.827384	3.496544	-1.656167	-0.837777	3.498971	-1.659037
C	-0.285272	4.239343	0.460671	-0.292354	4.245330	0.456414
H	1.136114	4.497714	-1.259700	1.124660	4.504957	-1.267664
C	-1.927469	3.230199	-0.800474	-1.937004	3.234008	-0.801214
H	-0.779784	3.265839	-2.713182	-0.792577	3.270107	-2.716412
C	-1.597199	3.674032	0.506478	-1.604283	3.679570	0.504868
H	0.232386	4.711759	1.286410	0.224533	4.722631	1.279734
H	-2.857337	2.761547	-1.093573	-2.867898	2.766283	-1.092443
H	-2.244585	3.624399	1.373200	-2.250452	3.632329	1.372564
C	-3.672058	-1.901877	-0.883927	-3.671267	-1.911905	-0.889092
C	-2.614404	-2.464808	-1.656167	-2.611309	-2.475022	-1.659037
C	-3.528743	-2.366724	0.460671	-3.530386	-2.375850	0.456414
H	-4.463191	-1.264953	-1.259700	-4.463737	-1.278494	-1.267664
C	-1.833700	-3.284337	-0.800474	-1.832231	-3.294498	-0.801214
H	-2.438407	-2.308232	-2.713182	-2.435707	-2.321445	-2.716412
C	-2.383206	-3.220231	0.506478	-2.384460	-3.229135	0.504868
H	-4.196696	-2.154628	1.286410	-4.202185	-2.166865	1.279734
H	-0.962902	-3.855300	-1.093573	-0.961722	-3.866814	-1.092443
H	-2.016529	-3.756068	1.373200	-2.020463	-3.765113	1.372564
C	3.483103	-2.229157	-0.883927	3.491392	-2.223458	-0.889092
C	3.441788	-1.031736	-1.656167	3.449087	-1.023949	-1.659037
C	3.814015	-1.872619	0.460671	3.822740	-1.869479	0.456414
H	3.327077	-3.232761	-1.259700	3.339077	-3.226462	-1.267664
C	3.761169	0.054138	-0.800474	3.769235	0.060490	-0.801214
H	3.218192	-0.957606	-2.713182	3.228284	-0.948662	-2.716412
C	3.980405	-0.453801	0.506478	3.988742	-0.450435	0.504868
H	3.964310	-2.557132	1.286410	3.977652	-2.555767	1.279734
H	3.820239	1.093752	-1.093573	3.829620	1.100531	-1.092443
H	4.261115	0.131668	1.373200	4.270915	0.132784	1.372564

Table S2 Coordinates of Cp₃Nb₃(CO)₉ 9-1 C₃

	BP86/SDD			BP86/LANL2DZ		
Nb	0.000000	1.973204	-0.010936	0.000000	1.973810	-0.009535
Nb	1.708845	-0.986602	-0.010936	1.709370	-0.986905	-0.009535
Nb	-1.708845	-0.986602	-0.010936	-1.709370	-0.986905	-0.009535
C	1.541260	-0.543208	2.046318	1.534206	-0.553585	2.051644
O	1.688052	-0.437658	3.207084	1.684259	-0.455102	3.212467
C	0.510835	-1.500784	-1.673679	0.519135	-1.503081	-1.678253
O	0.283556	-1.944379	-2.754461	0.290504	-1.942757	-2.759101
C	-1.241062	-1.063166	2.046318	-1.246522	-1.051868	2.051644
O	-1.223048	-1.243067	3.207084	-1.236259	-1.231060	3.212467
C	-1.555135	0.307996	-1.673679	-1.561274	0.301956	-1.678253
O	-1.825660	0.726623	-2.754461	-1.827729	0.719795	-2.759101
C	1.044300	1.192789	-1.673679	1.042139	1.201125	-1.678253
O	1.542104	1.217756	-2.754461	1.537225	1.222963	-2.759101
C	-0.300198	1.606374	2.046318	-0.287684	1.605454	2.051644
O	-0.465003	1.680724	3.207084	-0.448000	1.686162	3.212467
C	1.913452	2.368998	0.644690	1.914532	2.376159	0.642609
O	2.973371	2.728634	1.026390	2.973750	2.737092	1.023692
C	1.094886	-2.841597	0.644690	1.100548	-2.846112	0.642609
O	0.876381	-3.939332	1.026390	0.883516	-3.943889	1.023692
C	-3.008338	0.472599	0.644690	-3.015079	0.469954	0.642609
O	-3.849752	1.210697	1.026390	-3.857266	1.206797	1.023692
C	0.207753	4.177248	-0.914953	0.191369	4.183679	-0.920143
C	-0.820652	3.536435	-1.688776	-0.838680	3.539638	-1.690059
C	-0.273002	4.305310	0.440150	-0.284921	4.311488	0.437090
H	1.169328	4.531884	-1.294250	1.149286	4.542895	-1.303863
C	-1.933051	3.282645	-0.822793	-1.947764	3.284052	-0.819798
H	-0.770132	3.286799	-2.751414	-0.791999	3.291942	-2.753070
C	-1.598598	3.743664	0.491538	-1.609128	3.746391	0.493481
H	0.255431	4.779670	1.270936	0.243713	4.790663	1.264819
H	-2.872460	2.807623	-1.112011	-2.887244	2.807027	-1.105174
H	-2.249884	3.701357	1.368027	-2.256935	3.703505	1.372353
C	-3.721479	-1.908705	-0.914953	-3.718857	-1.926109	-0.920143
C	-2.652316	-2.478923	-1.688776	-2.646077	-2.496138	-1.690059
C	-3.592006	-2.389082	0.440150	-3.591397	-2.402492	0.437090
H	-4.509391	-1.253274	-1.294250	-4.508905	-1.276136	-1.303863
C	-1.876328	-3.315394	-0.822793	-1.870191	-3.328839	-0.819798
H	-2.461386	-2.310353	-2.751414	-2.454906	-2.331862	-2.753070
C	-2.442809	-3.256259	0.491538	-2.439905	-3.266741	0.493481
H	-4.267031	-2.168626	1.270936	-4.270693	-2.184270	1.264819
H	-0.995243	-3.891435	-1.112011	-0.987334	-3.903941	-1.105174
H	-2.080528	-3.799135	1.368027	-2.078862	-3.806316	1.372353
C	3.513726	-2.268543	-0.914953	3.527488	-2.257570	-0.920143
C	3.472968	-1.057512	-1.688776	3.484757	-1.043501	-1.690059
C	3.865009	-1.916228	0.440150	3.876318	-1.908995	0.437090
H	3.340062	-3.278610	-1.294250	3.359619	-3.266758	-1.303863
C	3.809379	0.032749	-0.822793	3.817955	0.044787	-0.819798
H	3.231518	-0.976446	-2.751414	3.246905	-0.960080	-2.753070
C	4.041407	-0.487405	0.491538	4.049033	-0.479649	0.493481
H	4.011601	-2.611045	1.270936	4.026980	-2.606393	1.264819
H	3.867703	1.083812	-1.112011	3.874579	1.096914	-1.105174
H	4.330411	0.097778	1.368027	4.335797	0.102811	1.372353

Table S3 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_9$ 9-2 C_1

	MPW1PW91/SDD			MPW1PW91/LANL2DZ		
Nb	-1.287701	-1.411223	-0.029670	-1.273498	-1.421744	-0.031545
Nb	1.926135	-0.269851	-0.005097	1.918526	-0.265242	-0.005214
Nb	-0.744079	1.791393	0.032875	-0.749103	1.791558	0.036803
C	-1.168189	0.029100	-1.665584	-1.163031	0.010346	-1.671556
C	-1.111893	0.530583	1.707912	-1.112071	0.538339	1.718376
C	2.218997	-2.305559	0.153603	2.220192	-2.301907	0.157756
C	-0.303881	-2.312734	1.573912	-0.286124	-2.308663	1.582761
C	-0.386422	-2.794155	-1.268278	-0.371191	-2.806661	-1.269049
C	1.402911	-0.777819	-1.995876	1.412215	-0.775318	-2.004252
C	1.481670	-0.326457	2.075276	1.483387	-0.304767	2.082462
C	0.631160	1.973809	-1.510748	0.626783	1.973991	-1.509898
C	0.711170	2.531107	1.282093	0.702824	2.551301	1.279863
O	-1.436860	0.248752	-2.792575	-1.428393	0.237591	-2.796060
O	-1.451545	0.352620	2.818604	-1.454898	0.350128	2.824839
O	2.521017	-3.419588	0.241598	2.528049	-3.413820	0.247594
O	0.054587	-2.967494	2.462028	0.072792	-2.955244	2.476276
O	-0.016265	-3.644655	-1.963406	-0.001056	-3.655968	-1.965445
O	1.359551	-1.052536	-3.116326	1.374463	-1.051327	-3.124068
O	1.451374	-0.353084	3.226246	1.455732	-0.319328	3.233330
O	1.223196	2.345908	-2.446383	1.215905	2.345935	-2.446873
O	1.430602	3.078283	2.017350	1.422027	3.104720	2.010178
C	3.712920	1.003414	1.010516	3.710431	1.018903	1.010527
C	4.181525	-0.310860	0.692892	4.181012	-0.296032	0.695262
C	3.418509	1.672088	-0.203750	3.416651	1.686315	-0.204751
H	3.627890	1.432541	2.001075	3.626392	1.449684	2.000415
C	4.165805	-0.443799	-0.729661	4.166928	-0.430657	-0.727251
H	4.539308	-1.047349	1.401554	4.543204	-1.029134	1.405091
C	3.680465	0.782880	-1.277409	3.679531	0.795008	-1.277043
H	3.049462	2.684445	-0.295636	3.047639	2.698496	-0.298110
H	4.501529	-1.303863	-1.295484	4.507396	-1.289525	-1.291950
H	3.559341	1.013621	-2.328358	3.562507	1.024792	-2.328598
C	-1.856234	3.758940	0.827254	-1.884821	3.768865	0.801572
C	-1.365340	4.023293	-0.487566	-1.395714	4.016606	-0.517355
C	-2.862832	2.761398	0.728796	-2.883298	2.761516	0.718786
H	-1.539614	4.249414	1.739523	-1.572309	4.276390	1.705881
C	-2.074064	3.178123	-1.395224	-2.099128	3.152408	-1.412104
H	-0.615085	4.757962	-0.752288	-0.654593	4.755854	-0.794378
C	-3.000232	2.406962	-0.642522	-3.018951	2.385486	-0.647497
H	-3.431028	2.360503	1.559234	-3.450118	2.370214	1.554694
H	-1.940302	3.135240	-2.469180	-1.966733	3.096298	-2.485526
H	-3.695479	1.684121	-1.049451	-3.711121	1.653426	-1.042825
C	-3.113615	-2.103074	1.341982	-3.105636	-2.105548	1.351238
C	-3.601460	-1.006162	0.585901	-3.596750	-1.017806	0.584271
C	-2.806923	-3.164187	0.429061	-2.797263	-3.176392	0.449319
H	-3.014608	-2.133815	2.419696	-3.006776	-2.125442	2.429222
C	-3.592574	-1.372924	-0.790264	-3.588722	-1.399817	-0.788488
H	-3.921977	-0.055727	0.991672	-3.920206	-0.064088	0.979533
C	-3.109268	-2.703435	-0.890060	-3.104060	-2.730965	-0.874193
H	-2.458823	-4.154552	0.693900	-2.449972	-4.164049	0.724887
H	-3.907528	-0.758994	-1.624359	-3.908653	-0.796107	-1.628095
H	-3.020114	-3.275412	-1.804953	-3.015709	-3.313082	-1.782745

Table S4 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_9$ 9-2 C_1

	BP86/SDD			BP86/LANL2DZ		
Nb	-1.303017	-1.423246	-0.007791	-1.280105	-1.441552	-0.008331
Nb	1.982146	-0.260575	-0.000491	1.975045	-0.245023	-0.000450
Nb	-0.778949	1.798994	0.011863	-0.796199	1.797081	0.012475
C	-1.144553	0.212983	-1.610534	-1.131751	0.197322	-1.610316
C	-1.142083	0.306615	1.621802	-1.135315	0.297881	1.622163
C	2.320109	-2.299015	0.022213	2.332821	-2.281997	0.022981
C	-0.319452	-2.534283	1.450748	-0.288240	-2.538234	1.456756
C	-0.338706	-2.617197	-1.406545	-0.308494	-2.624530	-1.411959
C	1.450628	-0.622961	-2.024431	1.463126	-0.608113	-2.033172
C	1.460999	-0.551217	2.038986	1.468397	-0.532582	2.047102
C	0.630113	2.202882	-1.455099	0.610238	2.213450	-1.455062
C	0.639765	2.307271	1.430981	0.616522	2.320088	1.433132
O	-1.463983	0.280825	-2.766271	-1.447457	0.262216	-2.765726
O	-1.475837	0.276216	2.774134	-1.467906	0.260139	2.773043
O	2.648023	-3.428970	0.034523	2.673040	-3.407945	0.035467
O	0.044331	-3.299271	2.270575	0.079810	-3.296359	2.280875
O	0.031442	-3.411236	-2.195046	0.066120	-3.412023	-2.204763
O	1.402628	-0.799559	-3.183467	1.422443	-0.783288	-3.192165
O	1.412900	-0.687625	3.202922	1.425530	-0.664097	3.211319
O	1.263375	2.654484	-2.349449	1.239235	2.668432	-2.350199
O	1.300595	2.785587	2.290220	1.272654	2.801256	2.293945
C	3.732839	0.998092	1.138924	3.722011	1.034598	1.140472
C	4.256989	-0.276815	0.716019	4.255886	-0.237196	0.717789
C	3.420663	1.760315	-0.031447	3.406151	1.795702	-0.029994
H	3.615190	1.340178	2.169951	3.603730	1.376136	2.171457
C	4.253395	-0.296535	-0.726259	4.253405	-0.256666	-0.724681
H	4.630222	-1.067008	1.371970	4.637259	-1.023103	1.373988
C	3.725605	0.965013	-1.181931	3.716375	1.001808	-1.180464
H	3.010750	2.771676	-0.044070	2.988882	2.803965	-0.042640
H	4.621781	-1.105300	-1.362028	4.630758	-1.061063	-1.360512
H	3.601101	1.277464	-2.221504	3.593102	1.314087	-2.220082
C	-1.913860	3.677525	1.050985	-1.961774	3.674442	1.042474
C	-1.390461	4.104592	-0.221280	-1.444976	4.098515	-0.233889
C	-2.930703	2.699387	0.807949	-2.966529	2.681709	0.808456
H	-1.602407	4.045097	2.032084	-1.652935	4.052821	2.020165
C	-2.095419	3.382931	-1.252047	-2.145006	3.362235	-1.258571
H	-0.625057	4.868650	-0.378051	-0.692718	4.873932	-0.397699
C	-3.041949	2.516285	-0.613060	-3.079053	2.488006	-0.611798
H	-3.515661	2.190761	1.578230	-3.545592	2.172743	1.582759
H	-1.942806	3.480392	-2.329749	-1.996996	3.455828	-2.337147
H	-3.733982	1.843643	-1.124856	-3.766158	1.805397	-1.116690
C	-3.150603	-2.366944	1.227309	-3.131800	-2.393216	1.231662
C	-3.655678	-1.160312	0.646317	-3.645089	-1.195239	0.640175
C	-2.811350	-3.267383	0.148609	-2.781750	-3.299472	0.160429
H	-3.056597	-2.572489	2.296078	-3.038133	-2.589600	2.302128
C	-3.637680	-1.305728	-0.783984	-3.624516	-1.352481	-0.789689
H	-3.995095	-0.282718	1.200729	-3.994381	-0.316300	1.185957
C	-3.122159	-2.602811	-1.094429	-3.098901	-2.648037	-1.088487
H	-2.437044	-4.288153	0.255284	-2.402734	-4.317495	0.275918
H	-3.957769	-0.562838	-1.517863	-3.951594	-0.618573	-1.529257
H	-3.006500	-3.021185	-2.096949	-2.978994	-3.074135	-2.087171

Table S5 Coordinates of Cp₃Nb₃(CO)₉ 9-3 C₁

	MPW1PW91/SDD			MPW1PW91/LANL2DZ		
C	-0.547471	0.457443	-1.722699	-0.523698	0.472066	-1.731520
C	-1.799988	-0.300991	1.580027	-1.826764	-0.286001	1.584008
C	2.903116	-1.530359	1.015008	2.876806	-1.556540	1.040709
C	-0.724145	-2.747079	1.644874	-0.777438	-2.752560	1.646662
C	0.654814	-2.449563	-0.652491	0.631642	-2.459748	-0.645314
C	2.706929	1.267780	1.267002	2.701759	1.239568	1.279460
C	0.819666	-0.463823	1.786272	0.785159	-0.490673	1.772817
C	0.636470	2.875614	-0.676524	0.694340	2.864239	-0.662996
C	-0.119224	2.052176	1.838476	-0.106851	2.043628	1.854308
O	-0.528235	0.155619	-2.862435	-0.509333	0.169735	-2.869461
O	-2.390206	-0.005559	2.543265	-2.419576	0.024560	2.539274
O	3.537530	-2.303159	1.593225	3.495475	-2.334048	1.629106
O	-0.577982	-3.450731	2.553608	-0.652759	-3.464917	2.551405
O	1.334697	-3.295109	-1.099802	1.298289	-3.315828	-1.089554
O	3.244319	1.992651	1.989030	3.236679	1.964956	2.002243
O	0.708930	-0.559777	2.945557	0.682172	-0.582401	2.934449
O	1.395717	3.679560	-1.041778	1.467599	3.657670	-1.020678
O	0.206198	2.438596	2.878973	0.208517	2.417613	2.901756
Nb	-0.922152	1.689257	-0.062821	-0.888752	1.699976	-0.063924
Nb	-1.123678	-1.578669	0.013035	-1.142788	-1.564958	0.018390
Nb	1.891875	-0.084149	-0.055760	1.888595	-0.108370	-0.052553
C	-2.829989	2.769363	0.912017	-2.797993	2.807695	0.899739
C	-2.040666	3.756490	0.245624	-1.988148	3.786484	0.244931
C	-3.354804	1.892202	-0.073988	-3.328056	1.943121	-0.094870
H	-3.015615	2.706104	1.977002	-2.995813	2.744620	1.962490
C	-2.075321	3.471047	-1.155091	-2.016067	3.508778	-1.157645
H	-1.538178	4.593915	0.713569	-1.479302	4.615242	0.721241
C	-2.885126	2.319124	-1.346874	-2.841143	2.369499	-1.361809
H	-4.010336	1.052926	0.117038	-3.998567	1.113615	0.086128
H	-1.604472	4.051872	-1.938191	-1.531670	4.087475	-1.934022
H	-3.116678	1.867442	-2.303622	-3.073325	1.927381	-2.322793
C	-2.937615	-3.157658	-0.065247	-2.983857	-3.122879	-0.104838
C	-3.496513	-1.901975	-0.421749	-3.522659	-1.854788	-0.449186
C	-1.987547	-3.514039	-1.065380	-2.028540	-3.477946	-1.100465
H	-3.202801	-3.745597	0.804699	-3.264365	-3.718687	0.754851
C	-2.912704	-1.490106	-1.653542	-2.923590	-1.434671	-1.671560
H	-4.260763	-1.376293	0.137819	-4.287292	-1.327981	0.108641
C	-1.972865	-2.475396	-2.049985	-1.992497	-2.426699	-2.071908
H	-1.404470	-4.426245	-1.092471	-1.458473	-4.397986	-1.135733
H	-3.144963	-0.587007	-2.201157	-3.140903	-0.521952	-2.208887
H	-1.373988	-2.452331	-2.951341	-1.387547	-2.401790	-2.968969
C	2.348320	0.829767	-2.304584	2.379141	0.796130	-2.309835
C	3.388289	1.220856	-1.415329	3.417737	1.171703	-1.411613
C	2.369892	-0.581454	-2.422798	2.378947	-0.615483	-2.426015
H	1.672902	1.496760	-2.820493	1.718780	1.473954	-2.831081
C	4.073145	0.040016	-0.993111	4.081499	-0.019094	-0.984026
H	3.645284	2.239492	-1.155189	3.689145	2.186275	-1.150297
C	3.426594	-1.077884	-1.612375	3.421338	-1.127509	-1.605892
H	1.694244	-1.176642	-3.021570	1.701748	-1.201206	-3.032179
H	4.953139	0.003520	-0.363230	4.955667	-0.068463	-0.346938
H	3.711572	-2.117920	-1.517849	3.689757	-2.171705	-1.508085

Table S6 Coordinates of Cp₃Nb₃(CO)₉ 9-3 C₁

	BP86/SDD			BP86/LANL2DZ		
C	-0.546458	0.139695	-1.552881	-0.529567	0.139738	-1.547078
C	-1.710787	-0.095550	1.495549	-1.708760	-0.073405	1.498346
C	2.875340	-1.529070	1.053294	2.847768	-1.558158	1.068174
C	-0.544170	-2.488666	1.758432	-0.579651	-2.479927	1.767470
C	0.625891	-2.549960	-0.663520	0.597436	-2.565409	-0.661637
C	2.806154	1.379297	1.130519	2.814943	1.355411	1.129443
C	0.997310	-0.149290	1.888444	0.988576	-0.155242	1.888428
C	0.632703	2.735339	-0.745620	0.677583	2.724149	-0.744305
C	-0.244720	2.270732	1.813190	-0.224375	2.279393	1.819887
O	-0.546296	0.008459	-2.758488	-0.536425	0.012643	-2.751276
O	-2.344920	0.049363	2.497408	-2.341161	0.078577	2.498740
O	3.475537	-2.332831	1.664721	3.430646	-2.370970	1.683766
O	-0.331194	-3.072664	2.758376	-0.381416	-3.061512	2.771695
O	1.335232	-3.412576	-1.073473	1.297144	-3.436298	-1.068218
O	3.364464	2.175812	1.790074	3.376023	2.153616	1.783871
O	0.847540	-0.187401	3.058314	0.845663	-0.190076	3.059390
O	1.381867	3.548593	-1.172001	1.436470	3.527065	-1.172269
O	0.047918	2.766997	2.838777	0.064839	2.772138	2.847929
Nb	-0.986845	1.662485	-0.036762	-0.959441	1.675954	-0.035654
Nb	-1.114305	-1.598719	-0.014998	-1.131134	-1.589472	-0.012780
Nb	1.930804	-0.065351	-0.052671	1.927110	-0.086752	-0.049900
C	-2.942041	2.896962	0.677226	-2.911351	2.943480	0.660602
C	-2.093116	3.782928	-0.079951	-2.047546	3.813120	-0.099519
C	-3.425494	1.886890	-0.216363	-3.404410	1.933093	-0.227228
H	-3.181550	2.980036	1.740178	-3.153909	3.038023	1.721791
C	-2.067603	3.311503	-1.444960	-2.025777	3.333097	-1.462186
H	-1.593160	4.677234	0.300078	-1.539948	4.705027	0.275754
C	-2.888293	2.143378	-1.524833	-2.860294	2.174649	-1.536474
H	-4.096612	1.069463	0.055764	-4.088642	1.127621	0.047287
H	-1.536942	3.779585	-2.277561	-1.487605	3.789494	-2.296299
H	-3.065355	1.556634	-2.429293	-3.043123	1.584331	-2.437259
C	-2.936026	-3.182323	0.281948	-2.984295	-3.152803	0.272936
C	-3.540593	-1.965852	-0.168343	-3.570889	-1.926137	-0.173472
C	-2.075451	-3.664788	-0.765373	-2.128284	-3.643378	-0.774810
H	-3.107834	-3.662743	1.248510	-3.162907	-3.633666	1.237907
C	-3.068112	-1.698823	-1.500665	-3.094275	-1.662083	-1.505768
H	-4.249085	-1.362849	0.405257	-4.273396	-1.316056	0.399681
C	-2.163704	-2.743568	-1.873803	-2.205081	-2.718372	-1.881825
H	-1.487833	-4.585837	-0.738550	-1.556019	-4.574065	-0.751515
H	-3.346459	-0.847993	-2.125890	-3.361112	-0.805605	-2.127934
H	-1.641999	-2.828447	-2.830006	-1.685538	-2.808771	-2.838478
C	2.356082	0.721304	-2.385175	2.378251	0.684057	-2.395946
C	3.430274	1.164046	-1.546420	3.454357	1.115223	-1.553435
C	2.376080	-0.708857	-2.422787	2.377303	-0.746636	-2.426288
H	1.645044	1.357527	-2.913236	1.677744	1.328353	-2.927988
C	4.126603	-0.003510	-1.060812	4.131808	-0.060097	-1.059010
H	3.692384	2.204630	-1.343296	3.730199	2.152729	-1.352909
C	3.463545	-1.163758	-1.608986	3.454516	-1.213275	-1.605044
H	1.675253	-1.337758	-2.973768	1.670498	-1.368483	-2.977189
H	5.025185	-0.006762	-0.439184	5.026744	-0.073368	-0.432402
H	3.751457	-2.206125	-1.455670	3.726892	-2.258846	-1.445327

Table S7 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_9$ 9-4 C_1

	MPW1PW91/SDD			MPW1PW91/LANL2DZ		
Nb	1.903336	-1.201949	0.085601	1.899745	-1.209711	0.087816
Nb	-2.263346	-0.717170	0.091430	-2.268640	-0.712772	0.094741
Nb	0.263638	1.712736	-0.111057	0.266190	1.714672	-0.106982
C	-2.057975	-0.515069	2.158922	-2.051329	-0.495212	2.162653
O	-2.056464	-0.549221	3.314568	-2.042899	-0.526786	3.318022
C	-1.335811	0.158489	-1.637271	-1.345049	0.148086	-1.639982
O	-1.282762	0.243965	-2.806210	-1.277904	0.228595	-2.806908
C	-0.240671	1.675633	1.922067	-0.220558	1.685009	1.932302
O	-0.450098	1.934046	3.031605	-0.426051	1.952199	3.040210
C	1.489983	0.563530	-1.466995	1.488382	0.559471	-1.462054
O	2.032459	0.699447	-2.518626	2.027071	0.692010	-2.513747
C	1.182652	-2.097322	-1.720919	1.179438	-2.103965	-1.724471
O	0.792904	-2.619945	-2.669060	0.788186	-2.624509	-2.672687
C	1.708032	-0.560869	2.145173	1.723201	-0.555782	2.146822
O	1.659269	-0.347059	3.274386	1.682600	-0.335181	3.274926
C	-0.264377	-1.505538	0.365234	-0.269350	-1.505662	0.375708
O	0.299330	-2.522324	0.798200	0.284564	-2.524219	0.809025
C	-3.211824	1.158703	0.247521	-3.212127	1.168745	0.246959
O	-3.827264	2.131096	0.383281	-3.823709	2.143147	0.381259
C	2.136149	2.040039	0.692421	2.143565	2.052123	0.686659
O	3.161998	2.357194	1.141608	3.172325	2.366072	1.129546
C	3.698429	-2.674002	-0.350921	3.700249	-2.682567	-0.360394
C	3.877695	-1.539973	-1.222359	3.872681	-1.545113	-1.230138
C	3.851119	-2.216641	0.982407	3.859960	-2.228544	0.972863
H	3.521077	-3.696708	-0.660102	3.524396	-3.705046	-0.671324
C	4.178000	-0.409033	-0.425592	4.178779	-0.416005	-0.432435
H	3.832965	-1.545284	-2.304702	3.824045	-1.548104	-2.312325
C	4.147678	-0.806113	0.929429	4.155738	-0.817326	0.921624
H	3.806489	-2.823572	1.878701	3.823496	-2.838270	1.867625
H	4.355585	0.593721	-0.790945	4.358455	0.586990	-0.796148
H	4.358904	-0.164966	1.776503	4.373222	-0.179143	1.769453
C	0.960912	3.641854	-1.282339	0.958311	3.638980	-1.303907
C	-0.033234	3.048288	-2.107667	-0.038408	3.041156	-2.123473
C	0.329207	4.069572	-0.069005	0.328986	4.077675	-0.092366
H	2.002168	3.776579	-1.547558	1.998521	3.772784	-1.573195
C	-1.269286	3.117158	-1.415650	-1.273161	3.117135	-1.429621
H	0.128780	2.601753	-3.080511	0.120843	2.590621	-3.094626
C	-1.053240	3.735442	-0.154925	-1.054020	3.744882	-0.173517
H	0.804405	4.594794	0.750524	0.805032	4.613313	0.719810
H	-2.219144	2.758824	-1.789793	-2.224431	2.758484	-1.799869
H	-1.810392	3.943365	0.590343	-1.809777	3.962036	0.570412
C	-4.191741	-1.417934	-1.119151	-4.201574	-1.430015	-1.115114
C	-3.136869	-2.278078	-1.535923	-3.146902	-2.294331	-1.524895
C	-4.427847	-1.654282	0.272762	-4.438500	-1.655537	0.278693
H	-4.735441	-0.729769	-1.754731	-4.746283	-0.747729	-1.755968
C	-2.725710	-3.046005	-0.413455	-2.736746	-3.054119	-0.395907
H	-2.719930	-2.336699	-2.533982	-2.731313	-2.363198	-2.522713
C	-3.515779	-2.665225	0.704169	-3.527802	-2.664051	0.718291
H	-5.193748	-1.188738	0.880928	-5.206358	-1.186791	0.881823
H	-1.934436	-3.785418	-0.403984	-1.946684	-3.794576	-0.380224
H	-3.453952	-3.089522	1.698797	-3.468293	-3.081909	1.715712

Table S8 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_9$ 9-4 C_1

	BP86/SDD			BP86/LANL2DZ		
Nb	1.951366	-1.175053	0.071287	1.947915	-1.181633	0.074691
Nb	-2.243675	-0.775301	0.099756	-2.246309	-0.772501	0.104196
Nb	0.203640	1.743333	-0.108927	0.204842	1.745479	-0.106559
C	-2.074738	-0.713467	2.175539	-2.066263	-0.697717	2.180535
O	-2.085720	-0.820271	3.346887	-2.071570	-0.803069	3.351739
C	-1.236998	0.233756	-1.578411	-1.239920	0.222321	-1.577999
O	-1.254095	0.266713	-2.775455	-1.242126	0.245687	-2.773644
C	-0.424142	1.634086	1.885160	-0.411698	1.644445	1.892181
O	-0.697166	1.875717	3.006633	-0.685436	1.894632	3.011323
C	1.563479	0.609579	-1.417571	1.559216	0.604548	-1.412998
O	2.140679	0.836132	-2.456277	2.132614	0.825363	-2.452824
C	1.282294	-2.040076	-1.773220	1.284146	-2.049193	-1.774438
O	0.914192	-2.559038	-2.755424	0.919434	-2.568066	-2.757528
C	1.650712	-0.540758	2.115938	1.660579	-0.533526	2.118282
O	1.550464	-0.347303	3.266047	1.565995	-0.332719	3.267478
C	-0.250646	-1.573714	0.342735	-0.253926	-1.577493	0.353922
O	0.363450	-2.602505	0.721169	0.350473	-2.608312	0.733334
C	-3.182760	1.102979	0.348856	-3.181814	1.110223	0.353445
O	-3.818151	2.078053	0.536218	-3.812434	2.087158	0.543703
C	2.033041	2.044879	0.822723	2.036110	2.061778	0.819031
O	3.042841	2.376675	1.343180	3.047569	2.392200	1.335592
C	3.783094	-2.641492	-0.333609	3.788860	-2.643822	-0.337935
C	3.991909	-1.478715	-1.182001	3.989620	-1.478954	-1.186795
C	3.881873	-2.205398	1.026301	3.892121	-2.208222	1.021585
H	3.619006	-3.667147	-0.673384	3.628503	-3.670086	-0.677600
C	4.251751	-0.349895	-0.344052	4.251797	-0.349782	-0.349433
H	3.988259	-1.464339	-2.275055	3.982361	-1.464446	-2.279750
C	4.173386	-0.780267	1.013093	4.179897	-0.781888	1.007836
H	3.798918	-2.834059	1.916913	3.817274	-2.838110	1.911965
H	4.437105	0.670620	-0.684858	4.435724	0.670995	-0.690057
H	4.342898	-0.149115	1.889069	4.352465	-0.151595	1.883838
C	0.935917	3.704389	-1.272849	0.929600	3.701799	-1.299334
C	-0.056926	3.113568	-2.120786	-0.064191	3.103758	-2.141374
C	0.281842	4.132515	-0.055895	0.276497	4.140643	-0.084703
H	1.993451	3.828097	-1.518725	1.986191	3.825718	-1.548287
C	-1.315128	3.180579	-1.437573	-1.321743	3.176102	-1.457068
H	0.119602	2.659725	-3.098672	0.111181	2.644036	-3.116318
C	-1.110984	3.802694	-0.162909	-1.116442	3.809507	-0.187535
H	0.754800	4.645611	0.785570	0.749178	4.665398	0.749511
H	-2.269553	2.816123	-1.823533	-2.276536	2.808211	-1.838692
H	-1.882033	4.000167	0.585513	-1.886736	4.014611	0.559390
C	-4.212791	-1.375271	-1.171238	-4.229166	-1.384597	-1.158544
C	-3.148528	-2.174277	-1.704660	-3.167227	-2.179397	-1.703122
C	-4.415046	-1.763642	0.205069	-4.417515	-1.775375	0.219322
H	-4.782588	-0.620883	-1.720093	-4.807967	-0.632406	-1.700590
C	-2.690967	-3.054383	-0.669159	-2.695931	-3.058574	-0.672464
H	-2.744351	-2.108680	-2.718047	-2.773034	-2.112007	-2.720048
C	-3.469004	-2.806689	0.511481	-3.464833	-2.815225	0.515933
H	-5.175114	-1.366884	0.883026	-5.174475	-1.383630	0.903500
H	-1.884307	-3.786161	-0.760096	-1.888255	-3.787812	-0.771924
H	-3.376432	-3.334482	1.464025	-3.363033	-3.345170	1.466205

Table S9 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_8$ 8-1 C_1

	MPW1PW91/SDD			MPW1PW91/LANL2DZ		
Nb	1.787955	-0.636188	-0.022264	1.741368	-0.730110	-0.025878
Nb	-0.341335	1.807377	-0.151191	-0.227591	1.817474	-0.145745
Nb	-1.563928	-1.166769	-0.081383	-1.625302	-1.079645	-0.082604
C	-1.048663	0.069905	-1.596976	-1.061944	0.130722	-1.609763
C	0.751922	-1.347709	1.665221	0.678168	-1.373571	1.672887
C	-1.680675	-0.185891	1.754688	-1.684491	-0.077748	1.743167
C	-3.280131	-0.079899	-0.382242	-3.278161	0.105641	-0.385048
C	1.544365	-0.416917	-2.116530	1.495778	-0.507417	-2.122938
C	1.656255	-2.601130	-0.592520	1.489875	-2.689842	-0.586515
C	1.461085	2.465979	-0.871765	1.604593	2.374639	-0.880855
C	0.689919	1.575176	1.608179	0.796708	1.538916	1.610801
O	-0.854285	0.934355	-2.405015	-0.841316	0.968554	-2.433480
O	0.559344	-1.835620	2.708551	0.458949	-1.841108	2.719151
O	-1.931986	0.192099	2.825290	-1.914916	0.318421	2.812176
O	-4.283472	0.460277	-0.607949	-4.246425	0.705549	-0.610803
O	1.600465	-0.395529	-3.268970	1.546582	-0.494256	-3.275494
O	1.740411	-3.710941	-0.930624	1.511972	-3.803781	-0.918284
O	2.408258	3.007487	-1.281720	2.576817	2.859727	-1.301064
O	1.168406	1.696635	2.668450	1.284895	1.635481	2.668459
C	4.086595	-1.084547	-0.410049	4.015576	-1.316022	-0.420080
C	3.945854	0.330597	-0.527086	3.960552	0.104728	-0.543199
C	3.796860	-1.439937	0.944122	3.712631	-1.647087	0.937452
H	4.401183	-1.760036	-1.196103	4.286554	-2.012560	-1.203894
C	3.586882	0.843726	0.747756	3.641276	0.644922	0.731462
H	4.112775	0.920681	-1.419662	4.159720	0.678840	-1.439438
C	3.481099	-0.243516	1.652446	3.473865	-0.430384	1.641910
H	3.844044	-2.435203	1.368571	3.703368	-2.641129	1.366975
H	3.425419	1.885013	0.989962	3.546100	1.695234	0.969704
H	3.220051	-0.168556	2.700811	3.225595	-0.335436	2.691565
C	-1.028202	3.946741	-0.891528	-0.794868	4.000277	-0.888365
C	-2.235006	3.184748	-0.818790	-2.045621	3.312531	-0.813073
C	-0.526655	4.088713	0.440433	-0.282783	4.112629	0.442481
H	-0.608393	4.390043	-1.785743	-0.353997	4.420787	-1.783452
C	-2.466291	2.848589	0.534704	-2.293985	2.990459	0.540685
H	-2.851965	2.894047	-1.660435	-2.681771	3.061684	-1.653191
C	-1.401717	3.379385	1.313744	-1.196850	3.455533	1.318030
H	0.350258	4.649741	0.738644	0.625244	4.622970	0.738562
H	-3.301687	2.279438	0.919032	-3.160321	2.469726	0.925372
H	-1.306355	3.299625	2.389417	-1.105321	3.372722	2.393708
C	-3.330470	-2.798387	0.161667	-3.488466	-2.612053	0.174597
C	-2.810383	-2.896729	-1.168786	-2.971089	-2.759738	-1.152851
C	-2.315467	-3.214432	1.065390	-2.502465	-3.074226	1.088477
H	-4.337267	-2.504866	0.433233	-4.476722	-2.255086	0.438570
C	-1.470490	-3.361602	-1.077778	-1.661203	-3.299987	-1.050291
H	-3.353212	-2.682527	-2.081219	-3.498315	-2.529218	-2.070427
C	-1.172565	-3.559651	0.305724	-1.379136	-3.495141	0.337729
H	-2.397984	-3.254773	2.144855	-2.591511	-3.095977	2.167789
H	-0.806071	-3.567342	-1.906988	-1.010961	-3.562652	-1.874490
H	-0.243024	-3.935895	0.709712	-0.475347	-3.921773	0.750456

Table S10 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_8$ 8-1 C_7

	BP86/SDD			BP86/LANL2DZ		
Nb	1.836295	-0.626207	-0.026669	1.787021	-0.725447	-0.032545
Nb	-0.362466	1.820372	-0.166315	-0.238476	1.831903	-0.158598
Nb	-1.585044	-1.185275	-0.058843	-1.649160	-1.094278	-0.058000
C	-1.095119	0.072363	-1.579176	-1.096788	0.134761	-1.587926
C	0.747347	-1.381272	1.620794	0.651726	-1.400040	1.618959
C	-1.693199	-0.203295	1.785955	-1.714736	-0.088111	1.773399
C	-3.327483	-0.120706	-0.314287	-3.323289	0.074208	-0.330426
C	1.532847	-0.420567	-2.106922	1.492384	-0.508393	-2.115385
C	1.733329	-2.590616	-0.616040	1.559546	-2.683822	-0.618241
C	1.436666	2.476434	-0.911071	1.595674	2.380169	-0.905915
C	0.676521	1.573680	1.597513	0.778623	1.542782	1.610642
O	-0.918893	0.936300	-2.422029	-0.894486	0.967675	-2.450569
O	0.583801	-1.899142	2.678117	0.462908	-1.895723	2.682164
O	-1.944483	0.176905	2.876419	-1.953365	0.314755	2.858703
O	-4.359662	0.418296	-0.512725	-4.317067	0.677512	-0.537009
O	1.564792	-0.402916	-3.280990	1.526655	-0.496071	-3.289166
O	1.825559	-3.716137	-0.968650	1.585245	-3.812796	-0.968482
O	2.389873	3.033213	-1.343246	2.578027	2.879285	-1.342438
O	1.146222	1.705057	2.682064	1.255751	1.644169	2.694111
C	4.178126	-1.036673	-0.374996	4.106282	-1.284328	-0.376669
C	4.008975	0.385847	-0.502008	4.029315	0.146385	-0.502091
C	3.870528	-1.396313	0.988093	3.776110	-1.624995	0.986371
H	4.511560	-1.716923	-1.162834	4.396178	-1.983577	-1.164947
C	3.615454	0.901347	0.776496	3.670757	0.685143	0.777756
H	4.171802	0.979747	-1.404830	4.229719	0.728918	-1.404497
C	3.516982	-0.194036	1.693258	3.501341	-0.403321	1.693299
H	3.923081	-2.399823	1.417957	3.764169	-2.630132	1.415053
H	3.423649	1.949454	1.011511	3.548159	1.743126	1.014153
H	3.230751	-0.121193	2.745348	3.221892	-0.313830	2.745607
C	-1.073968	3.978271	-0.910449	-0.824676	4.028835	-0.922413
C	-2.287118	3.204046	-0.817618	-2.083669	3.331026	-0.826228
C	-0.549994	4.128969	0.425528	-0.294867	4.159078	0.413357
H	-0.661263	4.419956	-1.820668	-0.386662	4.439360	-1.835316
C	-2.499326	2.867054	0.552525	-2.318935	3.018803	0.545858
H	-2.918616	2.902818	-1.657517	-2.731348	3.063350	-1.664965
C	-1.416182	3.410496	1.321355	-1.204739	3.500305	1.313205
H	0.340002	4.695117	0.710850	0.626016	4.674907	0.695705
H	-3.332066	2.285469	0.951738	-3.184471	2.487971	0.946194
H	-1.301525	3.332183	2.405114	-1.097648	3.425852	2.397836
C	-3.339035	-2.874484	0.129718	-3.505591	-2.680885	0.150010
C	-2.804521	-2.927598	-1.212353	-2.974605	-2.786043	-1.191305
C	-2.312526	-3.299138	1.036525	-2.507539	-3.155542	1.064427
H	-4.362066	-2.603797	0.403881	-4.509622	-2.342674	0.419580
C	-1.444817	-3.372276	-1.124979	-1.645138	-3.311432	-1.095761
H	-3.350159	-2.690734	-2.129340	-3.504802	-2.531185	-2.112412
C	-1.148183	-3.603623	0.267371	-1.363521	-3.540172	0.300661
H	-2.400866	-3.368246	2.123989	-2.600141	-3.203403	2.152414
H	-0.762006	-3.537696	-1.961196	-0.975906	-3.535792	-1.929031
H	-0.201963	-3.970851	0.667828	-0.441677	-3.959115	0.707445

Table S11 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_8$ 8-2 C_1

	MPW1PW91/SDD			MPW1PW91/LANL2DZ		
Nb	-1.609514	-0.910636	-0.103832	-1.600700	-0.915534	-0.100758
Nb	1.716603	-0.887900	-0.139555	1.716323	-0.878238	-0.138440
Nb	-0.038627	1.827883	0.062353	-0.046677	1.822758	0.061320
C	-0.058686	-0.108218	-1.259853	-0.057574	-0.109256	-1.267107
C	-0.002116	0.544329	1.766686	-0.007834	0.528508	1.756472
C	1.338944	2.456843	1.458471	1.320289	2.455813	1.468319
C	-1.697392	2.295123	1.165594	-1.711517	2.284127	1.159894
C	-1.377873	-2.413627	-1.490024	-1.346164	-2.436791	-1.467165
C	-2.599180	0.035359	-1.620451	-2.570096	0.011542	-1.643172
C	1.548363	-2.795825	-0.979511	1.604822	-2.771892	-1.027062
C	0.970852	-2.048635	1.376135	0.929389	-2.074478	1.329305
O	0.803413	-0.233527	-2.155079	0.790492	-0.219298	-2.171028
O	-0.017423	0.213954	2.895179	-0.018616	0.195017	2.884183
O	2.103469	2.835654	2.244249	2.082423	2.834352	2.255826
O	-2.619454	2.660769	1.769158	-2.638638	2.650825	1.754447
O	-1.347784	-3.236376	-2.303366	-1.303964	-3.272963	-2.265582
O	-3.173399	0.539676	-2.494306	-3.134217	0.506978	-2.528124
O	1.580253	-3.884501	-1.362468	1.660135	-3.847597	-1.440751
O	0.772962	-2.782823	2.259136	0.722544	-2.830185	2.191966
C	-3.707877	-1.959331	0.271490	-3.716650	-1.949496	0.269082
C	-2.743514	-2.693100	1.032554	-2.766031	-2.689150	1.041091
C	-3.820695	-0.655696	0.856999	-3.823107	-0.642827	0.848902
H	-4.297015	-2.341968	-0.552681	-4.299324	-2.329141	-0.561202
C	-2.268206	-1.843717	2.068782	-2.293714	-1.841735	2.080009
H	-2.455997	-3.725188	0.873833	-2.485713	-3.724088	0.887728
C	-2.937711	-0.597686	1.965881	-2.950971	-0.590341	1.967476
H	-4.497242	0.128924	0.541697	-4.490286	0.146345	0.525124
H	-1.519920	-2.096742	2.808443	-1.555357	-2.100262	2.827504
H	-2.798123	0.246478	2.627017	-2.811402	0.253382	2.628935
C	4.008201	-1.479009	-0.598798	4.040388	-1.472739	-0.504647
C	3.905318	-0.105715	-0.938983	3.938468	-0.110155	-0.886441
C	3.764806	-1.606891	0.804904	3.750293	-1.565685	0.892306
H	4.274914	-2.280888	-1.276031	4.334669	-2.290761	-1.150676
C	3.579135	0.622554	0.229858	3.568100	0.646033	0.251916
H	4.017173	0.303133	-1.936441	4.085416	0.273886	-1.889162
C	3.472583	-0.306570	1.317035	3.433608	-0.256226	1.360063
H	3.826230	-2.523174	1.379039	3.794282	-2.467084	1.491131
H	3.484889	1.696450	0.299025	3.468411	1.721022	0.289478
H	3.280537	-0.056090	2.352983	3.208057	0.018373	2.382945
C	1.021582	3.789163	-0.958034	1.017082	3.789565	-0.965251
C	0.984385	2.800200	-1.973619	0.976711	2.804778	-1.984360
C	-0.318489	4.130682	-0.612100	-0.322578	4.133004	-0.616406
H	1.914112	4.226228	-0.526060	1.911025	4.223354	-0.532667
C	-0.383090	2.548504	-2.284688	-0.391903	2.557429	-2.295174
H	1.833749	2.322234	-2.443893	1.824712	2.327914	-2.458092
C	-1.188812	3.363074	-1.454174	-1.195026	3.371567	-1.461688
H	-0.619408	4.886958	0.102191	-0.620969	4.889407	0.098852
H	-0.740270	1.857496	-3.036241	-0.751406	1.871750	-3.050488
H	-2.270018	3.419448	-1.475427	-2.276114	3.430877	-1.482028

Table S12 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_8$ 8-2 C_1

	BP86/SDD			BP86/LANL2DZ		
Nb	-1.527960	-1.055473	-0.106366	-1.529229	-1.047138	-0.105565
Nb	1.802067	-0.766313	-0.139754	1.797310	-0.772726	-0.144126
Nb	-0.201814	1.855506	0.064665	-0.192609	1.850989	0.068011
C	-0.033122	-0.082170	-1.259936	-0.034839	-0.079978	-1.265684
C	-0.065480	0.526101	1.748829	-0.070885	0.511783	1.744164
C	1.082847	2.592785	1.495341	1.104497	2.563957	1.501325
C	-1.905563	2.159732	1.161854	-1.892923	2.162370	1.170603
C	-1.134707	-2.553639	-1.469760	-1.135925	-2.545355	-1.470808
C	-2.556698	-0.206515	-1.658767	-2.540510	-0.187717	-1.664286
C	1.845215	-2.667500	-0.995598	1.855973	-2.662923	-1.024875
C	1.112049	-2.028268	1.330867	1.077196	-2.050395	1.299566
O	0.846405	-0.134199	-2.168567	0.826156	-0.122822	-2.186080
O	-0.051645	0.195252	2.898189	-0.057074	0.176840	2.892007
O	1.804887	3.034985	2.317566	1.838497	2.989826	2.321093
O	-2.874147	2.443390	1.775003	-2.860650	2.449769	1.782633
O	-1.027481	-3.404305	-2.275744	-1.027288	-3.396293	-2.275831
O	-3.161404	0.245655	-2.566610	-3.137700	0.270087	-2.573892
O	2.005740	-3.762376	-1.392233	2.017924	-3.752108	-1.435520
O	0.956973	-2.810877	2.207373	0.913800	-2.844175	2.164340
C	-3.540755	-2.317279	0.244074	-3.564284	-2.290803	0.237540
C	-2.513330	-2.943389	1.043532	-2.548966	-2.931980	1.040408
C	-3.802653	-1.013777	0.810774	-3.814805	-0.986899	0.808244
H	-4.068078	-2.770675	-0.598846	-4.089331	-2.733787	-0.612385
C	-2.149123	-2.027637	2.085553	-2.181623	-2.025916	2.089701
H	-2.111133	-3.949866	0.903778	-2.157103	-3.942193	0.898069
C	-2.947970	-0.848141	1.947210	-2.965974	-0.836694	1.951825
H	-4.551161	-0.298369	0.461347	-4.552654	-0.261480	0.456976
H	-1.382952	-2.191817	2.846274	-1.422240	-2.202740	2.854132
H	-2.908482	0.025495	2.599901	-2.920184	0.033508	2.608411
C	4.175512	-1.126070	-0.555906	4.195061	-1.168136	-0.472649
C	3.937143	0.242536	-0.900633	3.972072	0.185350	-0.882191
C	3.916921	-1.283089	0.855710	3.894952	-1.266070	0.935080
H	4.536412	-1.903279	-1.234116	4.569755	-1.974735	-1.107792
C	3.512425	0.937130	0.274019	3.515950	0.929476	0.250836
H	4.026228	0.667440	-1.904562	4.096268	0.569189	-1.898732
C	3.479503	-0.010903	1.367148	3.450051	0.026339	1.381369
H	4.053936	-2.200514	1.433601	4.006014	-2.160947	1.552458
H	3.311760	2.005700	0.348132	3.321406	2.001544	0.274794
H	3.231950	0.216340	2.406943	3.174848	0.296005	2.403738
C	0.681638	3.935354	-0.943797	0.702274	3.933877	-0.942831
C	0.746904	2.950807	-1.980453	0.753253	2.956725	-1.987326
C	-0.701029	4.149013	-0.609032	-0.677144	4.157663	-0.599370
H	1.531842	4.454846	-0.493526	1.559297	4.442295	-0.492735
C	-0.599742	2.571585	-2.312285	-0.598470	2.592000	-2.314934
H	1.651981	2.554638	-2.446381	1.652251	2.555080	-2.459901
C	-1.494257	3.305618	-1.475378	-1.482168	3.328383	-1.468550
H	-1.082660	4.869056	0.119067	-1.048438	4.876677	0.135004
H	-0.887100	1.848382	-3.077881	-0.896190	1.877135	-3.084253
H	-2.585541	3.256215	-1.504096	-2.573944	3.288997	-1.491851

Table S13 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_8$ 8-3 C_7

	MPW1PW91/SDD			MPW1PW91/LANL2DZ		
Nb	2.007116	0.104740	-0.015060	2.011619	0.105669	-0.014827
Nb	-0.963696	-1.493479	-0.045169	-0.964080	-1.487419	-0.039375
Nb	-1.018130	1.572739	-0.060991	-1.023061	1.571189	-0.065321
C	-0.507766	-1.980729	1.925648	-0.516043	-1.998137	1.928583
O	-0.316536	-2.344974	3.004757	-0.321694	-2.373462	3.002832
C	-1.900109	0.266500	-1.414548	-1.912662	0.274430	-1.422282
O	-2.572231	0.063862	-2.372271	-2.591214	0.066582	-2.371462
C	-1.295247	0.752838	1.808598	-1.314337	0.723344	1.788999
O	-1.604215	0.618294	2.927250	-1.632861	0.593393	2.906414
C	0.881906	2.217411	-0.712031	0.889955	2.219943	-0.686333
O	1.488987	3.085317	-1.244854	1.490590	3.097388	-1.208169
C	1.246466	-0.272295	-1.954152	1.251271	-0.272304	-1.956461
O	1.000051	-0.436792	-3.076924	1.004681	-0.434195	-3.078954
C	1.458310	0.424127	2.016285	1.457274	0.415209	2.019449
O	1.353411	0.580638	3.156063	1.342418	0.567403	3.158427
C	1.944411	-1.892051	0.461948	1.949337	-1.893573	0.456481
O	2.249849	-2.982068	0.756623	2.257866	-2.982454	0.749677
C	-2.883793	-1.154062	0.610789	-2.897108	-1.168354	0.601741
O	-3.982849	-1.041156	0.963098	-3.999349	-1.063969	0.943675
C	4.129698	-0.188752	-1.070258	4.141671	-0.174175	-1.075199
C	3.760813	1.187887	-1.190924	3.771222	1.203722	-1.183566
C	4.347864	-0.462398	0.308025	4.362371	-0.459243	0.300426
H	4.252192	-0.893952	-1.883288	4.267370	-0.870723	-1.894999
C	3.756660	1.756572	0.114166	3.768912	1.761552	0.126270
H	3.545154	1.719621	-2.108595	3.555560	1.742857	-2.096924
C	4.120559	0.733655	1.035359	4.133777	0.730631	1.038692
H	4.641911	-1.415208	0.730521	4.658248	-1.415200	0.714492
H	3.528497	2.785835	0.356730	3.543634	2.789177	0.377836
H	4.221808	0.849105	2.107804	4.237606	0.837758	2.111657
C	-1.172110	3.977997	0.191276	-1.172059	3.981948	0.224473
C	-1.688706	3.632968	-1.098363	-1.675221	3.662611	-1.077044
C	-2.014386	3.404751	1.169918	-2.029282	3.395915	1.183037
H	-0.291120	4.578988	0.378704	-0.290903	4.575709	0.433054
C	-2.856845	2.849903	-0.905732	-2.849897	2.882584	-0.912079
H	-1.262053	3.926888	-2.049739	-1.235914	3.970908	-2.018028
C	-3.055137	2.689177	0.495618	-3.065707	2.698336	0.483953
H	-1.895274	3.487834	2.243282	-1.922544	3.459628	2.259024
H	-3.488197	2.446476	-1.687499	-3.474450	2.496179	-1.707857
H	-3.870783	2.155107	0.968197	-3.890934	2.162466	0.937488
C	-2.298318	-2.947565	-1.371227	-2.289044	-2.950615	-1.378867
C	-1.123816	-2.700248	-2.131959	-1.115221	-2.694135	-2.138462
C	-1.913367	-3.667418	-0.194780	-1.901716	-3.674767	-0.205326
H	-3.303402	-2.664624	-1.656233	-3.295536	-2.673553	-1.664783
C	-0.020955	-3.271261	-1.442406	-0.010189	-3.264016	-1.451148
H	-1.079333	-2.148036	-3.062262	-1.073818	-2.143035	-3.069305
C	-0.499669	-3.862728	-0.245220	-0.486657	-3.863147	-0.256666
H	-2.579337	-4.042599	0.572449	-2.566771	-4.059980	0.557513
H	1.009630	-3.253001	-1.771096	1.019998	-3.241164	-1.780560
H	0.102919	-4.387057	0.484923	0.117490	-4.390076	0.470251

Table S14 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_8$ 8-3 C_1

	BP86/SDD			BP86/LANL2DZ		
Nb	-2.024733	-0.120548	-0.016279	2.031526	0.111635	-0.015377
Nb	0.957347	1.536232	-0.041453	-0.968188	-1.525174	-0.039209
Nb	1.019816	-1.597493	-0.067247	-1.014605	1.603110	-0.068896
C	0.573196	1.910858	1.967871	-0.596440	-1.927629	1.966720
O	0.423649	2.233881	3.087740	-0.448761	-2.264104	3.082510
C	1.804336	-0.215669	-1.442389	-1.815317	0.238302	-1.448264
O	2.408059	-0.011003	-2.467000	-2.428273	0.031370	-2.464263
C	1.355108	-0.823372	1.823252	-1.377307	0.797398	1.804256
O	1.685190	-0.709494	2.955997	-1.723103	0.686557	2.933253
C	-0.928416	-2.271174	-0.579723	0.949012	2.268234	-0.549619
O	-1.563320	-3.195888	-1.022970	1.581722	3.200094	-0.977508
C	-1.192211	0.264920	-1.926980	1.191100	-0.269540	-1.924789
O	-0.942261	0.436350	-3.070504	0.940133	-0.437204	-3.068187
C	-1.455605	-0.526123	1.998026	1.453343	0.496891	2.001483
O	-1.355805	-0.740724	3.148984	1.342828	0.697660	3.153631
C	-1.869727	1.862623	0.556524	1.869963	-1.872956	0.552062
O	-2.198044	2.947751	0.920956	2.192281	-2.958448	0.917849
C	2.884806	1.144607	0.578134	-2.906998	-1.148112	0.562684
O	4.008940	1.018582	0.913531	-4.033911	-1.026973	0.887635
C	-4.130853	0.181681	-1.193528	4.143903	-0.179423	-1.201989
C	-3.812619	-1.224668	-1.185113	3.831084	1.228223	-1.173525
C	-4.375803	0.587463	0.158099	4.389724	-0.604780	0.143714
H	-4.191216	0.824204	-2.075906	4.203264	-0.808643	-2.093699
C	-3.865524	-1.681549	0.174860	3.887341	1.666113	0.192806
H	-3.581876	-1.843053	-2.055256	3.602616	1.859160	-2.035112
C	-4.213784	-0.556799	1.003287	4.231898	0.528411	1.005557
H	-4.637132	1.595613	0.489273	4.647560	-1.618374	0.460539
H	-3.679743	-2.702934	0.513453	3.707590	2.683567	0.545845
H	-4.346231	-0.571708	2.088418	4.366572	0.528355	2.090317
C	1.251660	-4.029134	0.087380	-1.227736	4.040333	0.147780
C	1.721135	-3.620194	-1.212382	-1.663342	3.675199	-1.176895
C	2.113471	-3.458606	1.071528	-2.125914	3.452159	1.088813
H	0.381242	-4.660622	0.280217	-0.356664	4.655442	0.385239
C	2.881284	-2.797500	-1.024193	-2.837724	2.861331	-1.047411
H	1.267733	-3.889209	-2.170211	-1.177761	3.965372	-2.112366
C	3.123432	-2.685496	0.387164	-3.123718	2.711930	0.352808
H	2.027078	-3.582807	2.153940	-2.070012	3.543542	2.176422
H	3.481005	-2.343652	-1.816784	-3.418561	2.436563	-1.869665
H	3.942074	-2.135439	0.858775	-3.962399	2.158840	0.783808
C	2.282555	3.047375	-1.368977	-2.288173	-3.041367	-1.380011
C	1.081280	2.827808	-2.119558	-1.086757	-2.817418	-2.129882
C	1.922394	3.737047	-0.151283	-1.927896	-3.736591	-0.164709
H	3.289887	2.764688	-1.682721	-3.295883	-2.760886	-1.694275
C	-0.014501	3.382302	-1.380740	0.009306	-3.374411	-1.393056
H	1.012492	2.298326	-3.072890	-1.018739	-2.287741	-3.082803
C	0.497419	3.939407	-0.164995	-0.502227	-3.937350	-0.179568
H	2.612023	4.081234	0.623534	-2.617700	-4.087721	0.606538
H	-1.062194	3.373161	-1.688434	1.056812	-3.362741	-1.700860
H	-0.094240	4.435891	0.607250	0.089169	-4.438445	0.589705

Table S15 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_8$ 8-4 C_7

	MPW1PW91/SDD			MPW1PW91/LANL2DZ		
Nb	-1.511126	-1.294812	0.006743	-1.510505	-1.300717	0.018319
Nb	1.858298	-0.378572	-0.014184	1.850510	-0.369485	-0.010040
Nb	-0.688691	1.669446	0.023226	-0.700208	1.660489	0.025074
C	-1.167339	-3.309834	-0.261190	-1.185930	-3.304373	-0.361919
C	2.984239	1.305391	0.298878	2.964404	1.314033	0.375143
C	-1.155533	1.216100	-1.981706	-1.240371	1.255728	-1.982553
C	-0.683256	0.982563	1.998357	-0.579094	0.915247	1.973035
C	1.777323	-0.105229	2.080072	1.847682	-0.249250	2.108988
C	1.426287	0.800990	-1.680902	1.343014	0.884669	-1.601404
C	-0.460870	-1.850227	1.696360	-0.407913	-1.945936	1.639331
C	-0.561544	-1.442909	-1.830781	-0.596094	-1.387201	-1.841673
O	-0.998712	-4.450026	-0.412811	-1.022293	-4.434167	-0.577964
O	3.681764	2.220395	0.469424	3.643115	2.233741	0.584210
O	-1.497726	1.162708	-3.086423	-1.605699	1.219817	-3.078779
O	-0.816230	0.835859	3.143651	-0.653796	0.755531	3.122971
O	2.015204	0.032506	3.202125	2.138084	-0.206526	3.224972
O	1.600590	1.363561	-2.694185	1.535386	1.451452	-2.613413
O	-0.089598	-2.305959	2.703297	-0.017243	-2.453744	2.613913
O	-0.194980	-1.657317	-2.916143	-0.242253	-1.564668	-2.937495
C	-3.846044	-1.665030	-0.506391	-3.884568	-1.645285	-0.393723
C	-3.696047	-1.720349	0.923505	-3.667557	-1.721189	1.026670
C	-3.555378	-0.351285	-0.928135	-3.602860	-0.329533	-0.813016
C	-3.311927	-0.435963	1.372281	-3.249956	-0.446400	1.473979
C	-3.168699	0.410933	0.223166	-3.153974	0.413607	0.328678
C	0.077997	3.615348	1.170463	0.144483	3.580951	1.171460
C	0.715409	3.666930	-0.096907	0.700300	3.664762	-0.132909
C	-1.340064	3.695828	0.959818	-1.283218	3.675606	1.054354
C	-0.281842	3.760841	-1.097542	-0.359555	3.795765	-1.063502
C	-1.560328	3.784207	-0.452565	-1.592264	3.807113	-0.337111
C	2.831611	-1.870556	-1.641031	2.798779	-1.724675	-1.777079
C	3.853818	-1.067519	-1.053507	3.827587	-0.951451	-1.161983
C	2.302914	-2.713321	-0.628854	2.313385	-2.648495	-0.814814
C	3.945315	-1.416108	0.332825	3.968677	-1.401003	0.191055
C	2.973970	-2.431378	0.590634	3.018548	-2.447028	0.402148
H	-4.164724	-2.479460	-1.145422	-4.237020	-2.449705	-1.027808
H	-3.887713	-2.581639	1.551590	-3.838046	-2.589239	1.651521
H	-3.588300	0.009011	-1.948245	-3.682376	0.044790	-1.825443
H	-3.137160	-0.146758	2.400463	-3.031110	-0.169606	2.496863
H	-3.052143	1.506872	0.252467	-3.037265	1.509445	0.367339
H	0.578198	3.565750	2.129524	0.704206	3.498803	2.094575
H	1.782124	3.630312	-0.271965	1.752680	3.627605	-0.379722
H	-2.092140	3.760557	1.736965	-1.983930	3.724381	1.879107
H	-0.099906	3.818744	-2.163811	-0.246497	3.883522	-2.137144
H	-2.514454	3.912210	-0.950549	-2.576093	3.951743	-0.768535
H	2.519785	-1.853574	-2.677787	2.456600	-1.636755	-2.800359
H	4.482421	-0.359355	-1.578945	4.428475	-0.195782	-1.652416
H	1.518918	-3.446954	-0.761649	1.535372	-3.382578	-0.978434
H	4.659809	-1.025054	1.046653	4.702053	-1.055309	0.909080
H	2.794957	-2.919548	1.540964	2.877817	-3.008592	1.317649

Table S16 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_8$ 8-4 C_7

	BP86/SDD			BP86/LANL2DZ		
Nb	-1.621629	-1.189627	0.050438	-1.596428	-1.223175	0.053665
Nb	1.840118	-0.522781	0.017569	1.849210	-0.485918	0.028588
Nb	-0.544412	1.761688	0.001658	-0.590779	1.745237	-0.003130
C	-1.529930	-3.188728	-0.462028	-1.459903	-3.214279	-0.486642
C	3.138003	1.017344	0.457613	3.121113	1.077073	0.469980
C	-1.335176	1.471784	-1.932720	-1.371036	1.457143	-1.947275
C	-0.292636	0.762774	1.822916	-0.310959	0.733297	1.810091
C	2.002219	-0.658467	2.100695	2.014917	-0.625184	2.111417
C	1.211396	0.963922	-1.420473	1.183550	1.000518	-1.404974
C	-0.477462	-2.055668	1.548571	-0.431100	-2.084676	1.538362
C	-0.863747	-1.251602	-1.885896	-0.820961	-1.255639	-1.876962
O	-1.503389	-4.332448	-0.755397	-1.404989	-4.351915	-0.797465
O	3.911359	1.875471	0.704026	3.877579	1.949472	0.716354
O	-1.777013	1.514828	-3.022135	-1.802140	1.498109	-3.040184
O	-0.334355	0.628590	3.006326	-0.355677	0.608603	2.994811
O	2.345283	-0.811057	3.215170	2.362131	-0.780151	3.224055
O	1.564094	1.434016	-2.475438	1.540627	1.473508	-2.455568
O	-0.115067	-2.691148	2.480989	-0.052185	-2.722662	2.462191
O	-0.587744	-1.402256	-3.026000	-0.538733	-1.392815	-3.017214
C	-4.054458	-1.363345	-0.176762	-4.036898	-1.443804	-0.172072
C	-3.725269	-1.485486	1.230965	-3.706252	-1.556375	1.236392
C	-3.711590	-0.051270	-0.602997	-3.720189	-0.126140	-0.601709
C	-3.175600	-0.241154	1.666382	-3.180239	-0.301273	1.669605
C	-3.118348	0.641925	0.519203	-3.140990	0.580272	0.519899
C	0.453171	3.551302	1.306286	0.375007	3.553454	1.320833
C	1.014835	3.656336	-0.007395	0.944480	3.670057	0.010924
C	-0.968946	3.761356	1.201844	-1.048303	3.743403	1.207296
C	-0.042158	3.930285	-0.933812	-0.110733	3.933996	-0.921787
C	-1.278148	4.000940	-0.189008	-1.352154	3.984644	-0.184630
C	2.510833	-1.666306	-2.039465	2.551579	-1.599228	-2.050458
C	3.660109	-1.063422	-1.423109	3.685117	-0.974218	-1.427238
C	2.028376	-2.687977	-1.159435	2.093536	-2.640818	-1.180564
C	3.885793	-1.721981	-0.154148	3.926757	-1.640036	-0.164045
C	2.859977	-2.718846	0.009523	2.925509	-2.662694	-0.010803
H	-4.511778	-2.137461	-0.798493	-4.477087	-2.228918	-0.792394
H	-3.902976	-2.362880	1.858150	-3.866404	-2.436248	1.864687
H	-3.836807	0.349671	-1.611396	-3.854807	0.271031	-1.610204
H	-2.839681	-0.001050	2.677458	-2.852793	-0.050964	2.680653
H	-2.916592	1.732629	0.561574	-2.964034	1.674844	0.561492
H	1.005190	3.351701	2.227723	0.922279	3.354716	2.245156
H	2.069085	3.533679	-0.263921	2.002386	3.566036	-0.238321
H	-1.672350	3.782842	2.039238	-1.757648	3.751989	2.039761
H	0.074928	4.062812	-2.012238	0.011376	4.074591	-1.998461
H	-2.259703	4.246360	-0.604515	-2.334433	4.218968	-0.604649
H	2.079628	-1.393276	-3.004869	2.114326	-1.327430	-3.013159
H	4.276576	-0.275435	-1.862614	4.283931	-0.168849	-1.859241
H	1.167278	-3.334180	-1.341999	1.248918	-3.306399	-1.370480
H	4.708915	-1.529995	0.538685	4.746310	-1.436940	0.529721
H	2.748308	-3.396134	0.860123	2.831588	-3.352446	0.831705

Table S17 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_7$ 7-1 C_1

	MPW1PW91/SDD			MPW1PW91/LANL2DZ		
Nb	1.121988	1.451168	-0.153930	1.147492	1.428934	-0.155702
Nb	-1.931333	0.133905	-0.105171	-1.924864	0.164759	-0.106697
Nb	0.864113	-1.556695	-0.242616	0.833295	-1.567791	-0.246047
C	-0.363790	0.101630	-1.343556	-0.364141	0.109960	-1.359294
C	-0.256040	-1.639845	1.495446	-0.302299	-1.621475	1.483730
C	-0.523487	-2.736927	-1.206905	-0.578227	-2.728097	-1.208663
C	3.057051	0.838903	-0.400371	3.070818	0.781119	-0.432728
C	1.504865	0.712389	1.712341	1.527192	0.665366	1.702540
C	-2.405966	1.949526	-0.947259	-2.353450	1.989735	-0.959720
C	-1.441498	1.152460	1.634407	-1.406950	1.183056	1.625336
O	0.738613	0.057169	-1.954121	0.720902	0.052658	-1.986928
O	-0.673801	-1.919018	2.547578	-0.717789	-1.894093	2.538587
O	-1.226886	-3.500170	-1.730027	-1.294293	-3.479951	-1.728989
O	4.196361	0.642886	-0.549370	4.202863	0.563964	-0.599415
O	1.816888	0.438372	2.804042	1.835718	0.381762	2.792274
O	-2.737145	2.925305	-1.480457	-2.659749	2.968633	-1.500832
O	-1.415780	1.690849	2.665019	-1.368563	1.719737	2.656180
C	1.969255	3.414780	-1.177758	2.041372	3.398269	-1.144563
C	0.551039	3.531832	-1.283106	0.627233	3.549308	-1.259778
C	2.308352	3.477950	0.213268	2.369870	3.429932	0.250448
H	2.669530	3.356249	-2.001967	2.746669	3.341840	-1.964600
C	0.026015	3.660678	0.029292	0.093167	3.667203	0.049483
H	-0.024142	3.535746	-2.201303	0.061051	3.582772	-2.182902
C	1.101413	3.607914	0.952886	1.158841	3.572587	0.982268
H	3.307973	3.458230	0.629482	3.365355	3.382242	0.674447
H	-1.015565	3.783942	0.291936	-0.947986	3.808985	0.304499
H	1.014519	3.679249	2.030143	1.064702	3.632207	2.059536
C	-4.213028	-0.172106	-0.805838	-4.224261	-0.095578	-0.797998
C	-3.595135	-1.445102	-0.930400	-3.637453	-1.383192	-0.922174
C	-4.240660	0.171844	0.585334	-4.239221	0.252306	0.592646
H	-4.641813	0.406811	-1.614391	-4.641986	0.491566	-1.606487
C	-3.235623	-1.884995	0.372496	-3.284140	-1.828604	0.380794
H	-3.426532	-1.986343	-1.852805	-3.488511	-1.931299	-1.843798
C	-3.626180	-0.890878	1.309162	-3.648128	-0.823126	1.316834
H	-4.676855	1.066114	1.013284	-4.652961	1.157455	1.019982
H	-2.747522	-2.820828	0.612199	-2.817711	-2.775315	0.621388
H	-3.492164	-0.944030	2.382453	-3.512920	-0.877320	2.389819
C	2.163671	-3.389014	-1.018201	2.098978	-3.446617	-0.991363
C	3.087291	-2.326287	-0.820748	3.048661	-2.404145	-0.812780
C	1.612639	-3.734380	0.263419	1.539330	-3.755666	0.295878
H	1.953341	-3.883643	-1.958124	1.878239	-3.953080	-1.922619
C	3.124442	-2.019055	0.565506	3.093456	-2.073029	0.567668
H	3.660677	-1.828679	-1.593367	3.635319	-1.936675	-1.594211
C	2.210133	-2.874907	1.234159	2.156688	-2.892815	1.251665
H	0.925006	-4.544653	0.469476	0.832577	-4.545657	0.515840
H	3.742676	-1.269360	1.038876	3.731009	-1.331203	1.027664
H	2.030820	-2.893919	2.301752	1.977541	-2.889152	2.319375

Table S18 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_7$ 7-1 C_1

	BP86/SDD			BP86/LANL2DZ		
Nb	1.148790	1.458599	-0.156370	1.170859	1.439125	-0.158107
Nb	-1.942618	0.148130	-0.093856	-1.936873	0.173590	-0.096410
Nb	0.856671	-1.585623	-0.247768	0.831039	-1.594578	-0.252426
C	-0.356552	0.115853	-1.339043	-0.356720	0.122364	-1.354380
C	-0.294588	-1.618059	1.480937	-0.331120	-1.599543	1.470033
C	-0.535205	-2.748577	-1.225982	-0.584501	-2.738853	-1.224425
C	3.078765	0.815830	-0.395617	3.087717	0.763084	-0.425388
C	1.522990	0.721004	1.724354	1.544754	0.679390	1.714695
C	-2.412893	1.970424	-0.933185	-2.364471	2.002110	-0.948734
C	-1.440578	1.186038	1.637330	-1.410185	1.213863	1.625734
O	0.755290	0.066171	-1.974681	0.735151	0.066441	-2.011320
O	-0.705841	-1.910200	2.556312	-0.739232	-1.885334	2.548199
O	-1.248112	-3.520698	-1.769517	-1.310579	-3.501259	-1.762460
O	4.236309	0.604428	-0.543722	4.238898	0.532765	-0.588971
O	1.836384	0.451685	2.836137	1.856938	0.400038	2.823900
O	-2.749272	2.964828	-1.472830	-2.677630	2.998939	-1.496817
O	-1.424797	1.742705	2.681256	-1.383631	1.770878	2.668990
C	2.002472	3.427593	-1.216905	2.069710	3.415289	-1.181860
C	0.570537	3.551360	-1.306292	0.641689	3.571178	-1.284462
C	2.362971	3.503094	0.181367	2.416584	3.460250	0.221470
H	2.698817	3.351863	-2.056060	2.772742	3.341971	-2.015505
C	0.057858	3.695061	0.023330	0.116760	3.703284	0.040931
H	-0.022309	3.546888	-2.224945	0.059501	3.592841	-2.209563
C	1.154947	3.643281	0.942104	1.202278	3.610994	0.971671
H	3.376908	3.476378	0.588177	3.425324	3.406321	0.638407
H	-0.990366	3.821241	0.298752	-0.932081	3.844642	0.306283
H	1.081584	3.721395	2.029783	1.118982	3.676210	2.059314
C	-4.241458	-0.152372	-0.828692	-4.253911	-0.085052	-0.817983
C	-3.620632	-1.438712	-0.947333	-3.663316	-1.385836	-0.934181
C	-4.287767	0.193240	0.575385	-4.286423	0.267623	0.585036
H	-4.659452	0.436080	-1.649255	-4.661779	0.509369	-1.639315
C	-3.276707	-1.884096	0.371986	-3.323996	-1.833501	0.385819
H	-3.436634	-1.985037	-1.875472	-3.497892	-1.940317	-1.860780
C	-3.679739	-0.879763	1.312773	-3.700293	-0.816065	1.324353
H	-4.724589	1.100398	1.000754	-4.699923	1.186547	1.008263
H	-2.786069	-2.828129	0.618529	-2.852586	-2.786789	0.634452
H	-3.553282	-0.931000	2.396963	-3.570572	-0.865574	2.408041
C	2.166268	-3.450103	-1.006155	2.106398	-3.504427	-0.981214
C	3.101261	-2.382541	-0.796786	3.067424	-2.456907	-0.790587
C	1.588889	-3.790526	0.280185	1.521695	-3.809091	0.310775
H	1.959394	-3.948303	-1.956387	1.887841	-4.013311	-1.923113
C	3.121001	-2.068692	0.602305	3.096233	-2.119909	0.602815
H	3.693477	-1.884220	-1.568697	3.670773	-1.986993	-1.571575
C	2.182048	-2.923829	1.265602	2.135406	-2.939088	1.281355
H	0.881655	-4.598929	0.478966	0.795279	-4.596750	0.523158
H	3.741673	-1.311939	1.083887	3.735061	-1.369758	1.070693
H	1.979604	-2.936408	2.339136	1.933739	-2.928697	2.354888

Table S19 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_7$ 7-2 C_1

	MPW1PW91/SDD			MPW1PW91/LANL2DZ		
Nb	-1.672456	-0.742933	-0.151791	-1.687738	-0.704882	-0.148880
Nb	1.669630	-0.957732	-0.112532	1.650742	-0.986776	-0.116698
Nb	0.013196	1.804179	-0.218261	0.047430	1.798179	-0.221197
O	-1.914400	-0.140582	3.004448	-1.926598	-0.079670	3.004540
C	-1.766753	-0.312971	1.868726	-1.780319	-0.259687	1.870308
O	-4.185308	1.241465	-0.461614	-4.158544	1.326965	-0.502972
C	-3.228074	0.606213	-0.315151	-3.216748	0.673756	-0.340567
C	-1.665753	2.492234	0.748168	-1.624506	2.529052	0.734410
O	-2.499132	3.021647	1.361783	-2.449839	3.077947	1.340332
C	0.626479	1.375726	1.708822	0.648682	1.345718	1.705757
O	0.978404	1.304456	2.814624	1.000675	1.264906	2.810386
C	0.723478	-1.992210	1.403939	0.681589	-2.012821	1.391106
O	0.432155	-2.658243	2.315081	0.377417	-2.674050	2.301090
O	1.350879	-3.434246	-2.123770	1.250562	-3.428422	-2.156806
C	1.440566	-2.556542	-1.368282	1.369117	-2.564704	-1.389859
O	-0.756903	0.393659	-1.849449	-0.745382	0.392114	-1.871025
C	0.262432	-0.150827	-1.277644	0.257088	-0.157434	-1.286370
H	-4.005394	-1.526624	-1.996860	-4.053974	-1.470738	-1.972444
C	-3.330864	-1.995254	-1.291454	-3.382763	-1.943071	-1.266319
C	-2.103154	-2.648352	-1.609239	-2.172191	-2.625747	-1.587338
C	-3.556003	-2.155983	0.115471	-3.599374	-2.083196	0.144236
C	-1.575899	-3.200775	-0.418130	-1.646060	-3.176517	-0.394954
H	-1.645153	-2.702362	-2.589858	-1.725835	-2.702012	-2.571733
C	-2.453441	-2.880938	0.652221	-2.506750	-2.824783	0.680177
H	-4.423674	-1.817175	0.667753	-4.455148	-1.720264	0.699774
H	-0.655807	-3.761307	-0.329460	-0.736901	-3.754943	-0.308582
H	-2.319711	-3.172846	1.686550	-2.373127	-3.112289	1.715681
C	3.587243	0.133234	1.007752	3.606105	0.045960	1.022354
C	3.500966	-1.176967	1.533262	3.486832	-1.267978	1.532658
C	3.863527	0.039481	-0.387083	3.879350	-0.038769	-0.373992
H	3.468085	1.041253	1.584155	3.510275	0.950143	1.609079
C	3.724358	-2.096955	0.467695	3.686792	-2.180858	0.456250
H	3.305821	-1.431253	2.567738	3.285791	-1.529542	2.564141
C	3.956150	-1.338844	-0.725826	3.937811	-1.414877	-0.728184
H	4.015162	0.869116	-1.066291	4.058005	0.793940	-1.042690
H	3.758821	-3.175748	0.556243	3.692963	-3.261245	0.531861
H	4.215021	-1.741717	-1.697093	4.186497	-1.812595	-1.704281
C	0.862882	3.988578	0.168802	0.957014	3.959893	0.197823
C	1.953984	3.175121	-0.273857	2.028963	3.124215	-0.251468
C	-0.051779	4.122242	-0.921977	0.053339	4.134696	-0.896646
H	0.771560	4.465567	1.136653	0.874887	4.428012	1.170797
C	1.704485	2.811089	-1.628548	1.776851	2.784706	-1.611749
H	2.841362	2.940466	0.298479	2.906814	2.858905	0.321730
C	0.468863	3.395476	-2.019219	0.559000	3.407927	-2.001044
H	-0.974245	4.689078	-0.915449	-0.853180	4.726974	-0.887161
H	2.332213	2.191674	-2.256510	2.391751	2.157634	-2.244751
H	-0.016989	3.265928	-2.979589	0.078125	3.309438	-2.967501

Table S20 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_7$ 7-2 C_1

	BP86/SDD			BP86/LANL2DZ		
Nb	-1.732947	-0.678178	-0.150106	-1.744019	-0.648245	-0.148540
Nb	1.637275	-1.042347	-0.104841	1.624706	-1.063552	-0.108577
Nb	0.101815	1.824982	-0.217915	0.126855	1.816462	-0.221736
O	-1.943224	-0.064047	3.030845	-1.957906	-0.007592	3.027785
C	-1.800211	-0.238608	1.875468	-1.813833	-0.191642	1.874426
O	-4.165791	1.438972	-0.447025	-4.136131	1.507456	-0.497667
C	-3.220874	0.749661	-0.303866	-3.205797	0.803361	-0.335254
C	-1.551390	2.581691	0.755499	-1.520474	2.600687	0.744333
O	-2.370367	3.165703	1.375764	-2.332289	3.197750	1.360603
C	0.700829	1.350858	1.708273	0.712626	1.318586	1.703375
O	1.060969	1.273565	2.832319	1.069677	1.233343	2.827431
C	0.637477	-2.042123	1.407524	0.609425	-2.062052	1.394760
O	0.323199	-2.711552	2.334555	0.283766	-2.730022	2.318290
O	1.216935	-3.511997	-2.143531	1.139778	-3.504800	-2.167406
C	1.339521	-2.627340	-1.369563	1.286002	-2.631336	-1.385445
O	-0.761074	0.437601	-1.856816	-0.746380	0.425819	-1.884352
C	0.241506	-0.166683	-1.269284	0.239376	-0.175470	-1.278645
H	-4.113672	-1.362779	-2.020512	-4.151732	-1.324370	-1.998258
C	-3.454936	-1.870430	-1.311916	-3.496570	-1.832611	-1.286872
C	-2.242660	-2.576557	-1.634477	-2.299987	-2.565273	-1.609269
C	-3.690968	-2.030968	0.106377	-3.725099	-1.970115	0.135137
C	-1.734296	-3.159821	-0.434206	-1.792984	-3.142717	-0.405668
H	-1.780383	-2.643309	-2.623295	-1.847613	-2.653529	-2.600769
C	-2.607597	-2.806245	0.646543	-2.650660	-2.757331	0.677851
H	-4.550455	-1.651949	0.664614	-4.572852	-1.567521	0.694683
H	-0.824225	-3.754699	-0.345822	-0.893228	-3.752903	-0.316729
H	-2.484300	-3.107983	1.689648	-2.527213	-3.050810	1.723140
C	3.624088	-0.032267	1.021919	3.639412	-0.098211	1.037242
C	3.491991	-1.357807	1.535396	3.488342	-1.429418	1.531287
C	3.884601	-0.118245	-0.389927	3.894347	-0.167405	-0.376829
H	3.538034	0.880088	1.615765	3.566876	0.807199	1.643358
C	3.673792	-2.278682	0.446459	3.653554	-2.336698	0.428303
H	3.289929	-1.621232	2.576525	3.283789	-1.705492	2.568532
C	3.922181	-1.506867	-0.751090	3.910880	-1.551007	-0.758244
H	4.063484	0.721915	-1.065585	4.088214	0.679380	-1.039652
H	3.661843	-3.369037	0.518816	3.623036	-3.427710	0.484034
H	4.154938	-1.910271	-1.739645	4.134572	-1.942857	-1.753488
C	1.065428	3.986452	0.169254	1.122890	3.963766	0.202295
C	2.121850	3.111714	-0.284063	2.172483	3.080919	-0.252196
C	0.143533	4.166738	-0.925116	0.216924	4.173492	-0.900777
H	0.999699	4.465258	1.149230	1.054194	4.431506	1.187278
C	1.845745	2.759908	-1.650768	1.906659	2.750769	-1.626023
H	3.006965	2.831325	0.289794	3.047039	2.779945	0.327281
C	0.625812	3.409860	-2.036958	0.700010	3.423536	-2.017219
H	-0.759814	4.781137	-0.910130	-0.677171	4.801515	-0.887850
H	2.444237	2.102487	-2.286286	2.503441	2.093874	-2.263541
H	0.124138	3.304969	-3.003518	0.210146	3.341899	-2.991888

Table S21 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_7$ 7-3 C_3

	MPW1PW91/SDD			MPW1PW91/LANL2DZ		
Nb	0.000000	1.730850	0.060310	0.000000	1.724313	0.059678
Nb	1.498960	-0.865425	0.060310	1.493299	-0.862157	0.059678
Nb	-1.498960	-0.865425	0.060310	-1.493299	-0.862157	0.059678
C	0.000000	0.000000	1.660945	0.000000	0.000000	1.668050
C	-0.661385	-1.607260	-1.651348	-0.653419	-1.615858	-1.647484
C	-0.914610	-2.598060	0.985908	-0.917725	-2.601890	0.987677
C	-1.792681	2.091105	0.985908	-1.794440	2.095718	0.987677
C	-1.061235	1.376406	-1.651348	-1.072664	1.373806	-1.647484
C	2.707291	0.506955	0.985908	2.712165	0.506172	0.987677
C	1.722621	0.230854	-1.651348	1.726083	0.242051	-1.647484
O	0.000000	0.000000	2.844327	0.000000	0.000000	2.848905
O	-0.405912	-2.088635	-2.683950	-0.402100	-2.098659	-2.679998
O	-0.750259	-3.612030	1.534781	-0.758806	-3.616414	1.535366
O	-2.752980	2.455759	1.534781	-2.752503	2.465352	1.535366
O	-1.605855	1.395848	-2.683950	-1.616442	1.397559	-2.679998
O	3.503240	1.156271	1.534781	3.511309	1.151062	1.535366
O	2.011767	0.692787	-2.683950	2.018542	0.701100	-2.679998
C	0.225006	3.986917	0.949599	0.232121	3.990765	0.945854
C	1.529035	3.436978	0.997016	1.536877	3.441537	0.996387
C	-0.173540	4.064121	-0.421752	-0.165033	4.064422	-0.426313
H	-0.354568	4.319002	1.802177	-0.347327	4.326793	1.797035
C	1.945392	3.171518	-0.336476	1.953981	3.171481	-0.335769
H	2.104908	3.242088	1.893074	2.112328	3.252690	1.893919
C	0.895820	3.556077	-1.215700	0.904643	3.553223	-1.217491
H	-1.105292	4.472679	-0.793383	-1.095725	4.473242	-0.800333
H	2.902084	2.763421	-0.634676	2.911534	2.764086	-0.632318
H	0.920044	3.497362	-2.296779	0.930567	3.493174	-2.298397
C	3.340268	-2.188319	0.949599	3.340044	-2.196405	0.945854
C	2.211993	-3.042672	0.997016	2.212021	-3.051743	0.996387
C	3.606402	-1.881770	-0.421752	3.602409	-1.889289	-0.426313
H	3.917650	-1.852436	1.802177	3.920777	-1.862603	1.797035
C	1.773919	-3.270518	-0.336476	1.769593	-3.277937	-0.335769
H	1.755277	-3.443948	1.893074	1.760748	-3.455675	1.893919
C	2.631744	-2.553841	-1.215700	2.624859	-2.560055	-1.217491
H	4.426100	-1.279129	-0.793383	4.421803	-1.287695	-0.800333
H	0.942151	-3.894989	-0.634676	0.938002	-3.903506	-0.632318
H	2.568783	-2.545463	-2.296779	2.559894	-2.552481	-2.298397
C	-3.565274	-1.798598	0.949599	-3.572165	-1.794360	0.945854
C	-3.741028	-0.394306	0.997016	-3.748897	-0.389795	0.996387
C	-3.432862	-2.182351	-0.421752	-3.437376	-2.175133	-0.426313
H	-3.563081	-2.466566	1.802177	-3.573449	-2.464191	1.797035
C	-3.719311	0.099000	-0.336476	-3.723573	0.106456	-0.335769
H	-3.860185	0.201859	1.893074	-3.873076	0.202985	1.893919
C	-3.527563	-1.002236	-1.215700	-3.529503	-0.993167	-1.217491
H	-3.320808	-3.193551	-0.793383	-3.326078	-3.185546	-0.800333
H	-3.844235	1.131568	-0.634676	-3.849536	1.139420	-0.632318
H	-3.488827	-0.951900	-2.296779	-3.490461	-0.940693	-2.298397

Table S22 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_7$ 7-3 C_3

	BP86/SDD			BP86/LANL2DZ		
Nb	0.000000	1.748223	0.061060	0.000000	1.742749	1.742749
Nb	1.514006	-0.874112	0.061060	1.509265	-0.871374	-0.871374
Nb	-1.514006	-0.874112	0.061060	-1.509265	-0.871374	-0.871374
C	0.000000	0.000000	1.632195	0.000000	0.000000	0.000000
C	-0.651586	-1.602425	-1.654757	-0.645583	-1.609344	-1.609344
C	-0.898209	-2.591844	1.004333	-0.900003	-2.594572	-2.594572
C	-1.795498	2.073793	1.004333	-1.796964	2.076712	2.076712
C	-1.061948	1.365503	-1.654757	-1.070942	1.363763	1.363763
C	2.693707	0.518050	1.004333	2.696967	0.517860	0.517860
C	1.713534	0.236922	-1.654757	1.716524	0.245581	0.245581
O	0.000000	0.000000	2.841039	0.000000	0.000000	0.000000
O	-0.398474	-2.096433	-2.704711	-0.395344	-2.103596	-2.103596
O	-0.727236	-3.612483	1.581030	-0.733329	-3.616106	-3.616106
O	-2.764884	2.436047	1.581030	-2.764975	2.443134	2.443134
O	-1.616327	1.393305	-2.704711	-1.624096	1.394176	1.394176
O	3.492120	1.176437	1.581030	3.498304	1.172972	1.172972
O	2.014801	0.703128	-2.704711	2.019440	0.709420	0.709420
C	0.205693	4.036847	0.946202	0.211979	4.041974	4.041974
C	1.524099	3.487780	1.002417	1.532058	3.495423	3.495423
C	-0.189993	4.109208	-0.438832	-0.184312	4.110734	4.110734
H	-0.388103	4.366702	1.802526	-0.381101	4.374225	4.374225
C	1.951421	3.217343	-0.340681	1.958681	3.221223	3.221223
H	2.101237	3.291834	1.909440	2.109554	3.304257	3.304257
C	0.894054	3.598463	-1.233471	0.899809	3.598351	3.598351
H	-1.134637	4.507134	-0.818423	-1.129171	4.507202	4.507202
H	2.918829	2.805904	-0.635503	2.926417	2.810362	2.810362
H	0.920079	3.529891	-2.323803	0.925834	3.527638	3.527638
C	3.393166	-2.196559	0.946202	3.394463	-2.204566	-2.204566
C	2.258457	-3.063799	1.002417	2.261096	-3.074512	-3.074512
C	3.653675	-1.890065	-0.438832	3.652156	-1.895748	-1.895748
H	3.975726	-1.847244	1.802526	3.978741	-1.857070	-1.857070
C	1.810590	-3.298651	-0.340681	1.810321	-3.306879	-3.306879
H	1.800194	-3.465642	1.909440	1.806794	-3.479056	-3.479056
C	2.669333	-2.573505	-1.233471	2.666359	-2.578433	-2.578433
H	4.470611	-1.270942	-0.818423	4.467937	-1.275711	-1.275711
H	0.970570	-3.930732	-0.635503	0.970636	-3.939533	-3.939533
H	2.596936	-2.561757	-2.323803	2.592107	-2.565615	-2.565615
C	-3.598859	-1.840288	0.946202	-3.606442	-1.837408	-1.837408
C	-3.782556	-0.423981	1.002417	-3.793154	-0.420911	-0.420911
C	-3.463682	-2.219143	-0.438832	-3.467843	-2.214986	-2.214986
H	-3.587624	-2.519458	1.802526	-3.597640	-2.517156	-2.517156
C	-3.762011	0.081309	-0.340681	-3.769002	0.085656	0.085656
H	-3.901430	0.173807	1.909440	-3.916348	0.174799	0.174799
C	-3.563387	-1.024958	-1.233471	-3.566168	-1.019918	-1.019918
H	-3.335974	-3.236192	-0.818423	-3.338766	-3.231492	-3.231492
H	-3.889399	1.124828	-0.635503	-3.897054	1.129171	1.129171
H	-3.517015	-0.968134	-2.323803	-3.517941	-0.962023	-0.962023

Table S23 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_6$ 6-1 C_1

	MPW1PW91/SDD			MPW1PW91/LANL2DZ		
Nb	-1.626339	-0.761795	-0.041026	-1.631497	-0.750751	-0.043448
Nb	-0.007774	1.576518	-0.013410	-0.003449	1.567461	-0.012088
Nb	1.593033	-0.721613	-0.003515	1.593168	-0.719472	-0.000826
C	0.591062	0.976331	-1.847308	0.595197	0.971417	-1.851280
O	0.865678	0.840364	-2.983379	0.867686	0.845127	-2.987644
C	1.703549	0.828064	1.411206	1.698690	0.818558	1.432783
O	2.184333	1.388031	2.333552	2.168898	1.372251	2.361628
C	1.253911	-1.684289	1.816738	1.253095	-1.706311	1.809393
O	1.105428	-2.194547	2.841825	1.099304	-2.229289	2.826680
C	0.026005	-2.170178	-0.573385	0.020952	-2.153464	-0.598288
O	0.060612	-3.266666	-1.041586	0.052486	-3.237662	-1.088742
C	-1.993713	0.815813	-1.329510	-2.016640	0.831621	-1.322931
O	-2.581881	1.450490	-2.130772	-2.601268	1.471556	-2.120021
C	-1.393689	0.324884	1.666661	-1.394001	0.328967	1.671982
O	-1.457469	0.788438	2.747116	-1.458558	0.782787	2.755172
C	-3.753594	-1.479211	-0.933098	-3.767762	-1.484753	-0.924007
C	-2.932430	-2.632284	-0.885332	-2.938704	-2.632893	-0.887920
C	-3.959013	-1.027124	0.404521	-3.965741	-1.039819	0.417185
H	-4.154993	-1.016220	-1.826482	-4.179861	-1.021667	-1.812530
C	-2.632855	-2.905424	0.484134	-2.626815	-2.910213	0.477875
H	-2.574390	-3.203212	-1.733103	-2.586282	-3.198615	-1.741439
C	-3.273226	-1.921354	1.279385	-3.267508	-1.933569	1.282740
H	-4.557315	-0.175096	0.705166	-4.567905	-0.193516	0.726394
H	-2.026070	-3.726328	0.845805	-2.014463	-3.730239	0.832232
H	-3.253615	-1.861098	2.360911	-3.241643	-1.879661	2.364469
C	0.656252	3.774466	-0.778707	0.675545	3.773957	-0.772353
C	-0.757763	3.671202	-0.925614	-0.737779	3.673725	-0.932054
C	0.959425	3.724217	0.608176	0.965847	3.724167	0.617102
H	1.369737	3.876635	-1.587696	1.397056	3.874128	-1.574515
C	-1.322065	3.572037	0.381087	-1.314420	3.578586	0.369836
H	-1.306138	3.679175	-1.859001	-1.277597	3.686440	-1.870371
C	-0.262120	3.599502	1.326992	-0.263013	3.603730	1.325150
H	1.947400	3.753510	1.050752	1.950059	3.753166	1.068083
H	-2.377092	3.476322	0.609872	-2.372111	3.492521	0.589637
H	-0.359841	3.513865	2.402522	-0.370995	3.524507	2.400187
C	3.065785	-2.544817	-0.565816	3.061691	-2.545893	-0.603725
C	2.871602	-1.763046	-1.736500	2.886058	-1.726586	-1.751188
C	3.767698	-1.741455	0.384766	3.763962	-1.779049	0.377223
H	2.732268	-3.565462	-0.425521	2.717163	-3.566910	-0.497293
C	3.453449	-0.480732	-1.509134	3.479007	-0.456926	-1.479133
H	2.365105	-2.083680	-2.638633	2.386891	-2.013756	-2.668494
C	4.001244	-0.468535	-0.196473	4.016006	-0.491182	-0.162418
H	4.076509	-2.047803	1.377233	4.062325	-2.119832	1.361676
H	3.463289	0.341571	-2.213836	3.509567	0.384999	-2.159593
H	4.508706	0.363055	0.277281	4.530326	0.319087	0.339951

Table S24 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_6$ 6-1 C_1

	BP86/SDD			BP86/LANL2DZ		
Nb	-1.633344	-0.797644	-0.036576	-1.636452	-0.790810	-0.038008
Nb	-0.036603	1.600027	-0.018157	-0.034957	1.590313	-0.017572
Nb	1.613022	-0.715548	-0.022259	1.615222	-0.707773	-0.021274
C	0.600226	0.932801	-1.832305	0.597789	0.933060	-1.839937
O	0.900360	0.762561	-2.978945	0.894706	0.773232	-2.987425
C	1.693263	0.933832	1.340776	1.689131	0.927591	1.359106
O	2.257956	1.500294	2.239637	2.238928	1.489730	2.267193
C	1.253688	-1.578130	1.839886	1.256209	-1.589280	1.833298
O	1.104624	-2.042984	2.909256	1.103391	-2.061722	2.898321
C	0.063667	-2.179114	-0.590324	0.060780	-2.160496	-0.617093
O	0.096334	-3.291484	-1.069276	0.095697	-3.260442	-1.118478
C	-2.032182	0.769660	-1.338340	-2.056708	0.779257	-1.331403
O	-2.638792	1.404813	-2.153791	-2.661534	1.418884	-2.142206
C	-1.390334	0.338577	1.651251	-1.388912	0.337779	1.657877
O	-1.462193	0.825158	2.743893	-1.460892	0.813991	2.753622
C	-3.785414	-1.570044	-0.897435	-3.793009	-1.587409	-0.889237
C	-2.934662	-2.718579	-0.858712	-2.932971	-2.729558	-0.856260
C	-3.976523	-1.111932	0.453069	-3.980441	-1.131832	0.462796
H	-4.214224	-1.113818	-1.793657	-4.230822	-1.134961	-1.782997
C	-2.597914	-2.978884	0.516632	-2.586272	-2.988069	0.516922
H	-2.577155	-3.290499	-1.718711	-2.577037	-3.297901	-1.719082
C	-3.245897	-1.991243	1.327013	-3.237730	-2.005880	1.331959
H	-4.584854	-0.257391	0.762661	-4.593298	-0.282072	0.776516
H	-1.960992	-3.791987	0.873562	-1.942364	-3.797025	0.870725
H	-3.203295	-1.920767	2.417150	-3.190579	-1.937180	2.421960
C	0.555220	3.820417	-0.865974	0.579501	3.822381	-0.847783
C	-0.872381	3.683009	-0.958283	-0.846154	3.684650	-0.975581
C	0.913347	3.805644	0.521469	0.903207	3.807182	0.547868
H	1.242247	3.917678	-1.711021	1.287544	3.919561	-1.675302
C	-1.392165	3.596445	0.381155	-1.398938	3.599534	0.350761
H	-1.459149	3.654766	-1.879444	-1.410034	3.660241	-1.910955
C	-0.288893	3.666843	1.294968	-0.318263	3.668828	1.291396
H	1.925260	3.864067	0.930144	1.904943	3.865428	0.980700
H	-2.445530	3.483045	0.652665	-2.459025	3.491095	0.596196
H	-0.345178	3.600185	2.384634	-0.401728	3.604411	2.379392
C	3.135320	-2.566890	-0.478606	3.136702	-2.567206	-0.507220
C	2.971051	-1.816080	-1.689947	2.988486	-1.786327	-1.701455
C	3.806387	-1.722444	0.476813	3.807260	-1.751036	0.473555
H	2.801202	-3.594352	-0.314881	2.793386	-3.595477	-0.370406
C	3.541694	-0.511149	-1.482040	3.567655	-0.490466	-1.457429
H	2.493832	-2.173364	-2.606091	2.517661	-2.117297	-2.630530
C	4.050259	-0.454216	-0.140575	4.065984	-0.469879	-0.110933
H	4.086016	-1.998431	1.497205	4.076840	-2.054061	1.488955
H	3.566076	0.298153	-2.216291	3.609145	0.335092	-2.172428
H	4.536854	0.404421	0.329623	4.556815	0.372858	0.382799

TableS25 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_6$ 6-2 C_1

	MPW1PW91/SDD			MPW1PW91/LANL2DZ		
C	1.747212	0.192466	-1.891929	1.762459	0.189377	-1.906885
O	1.758283	0.706675	-2.950909	1.781400	0.715350	-2.957660
C	1.154763	0.401543	1.846356	1.134835	0.385697	1.862752
O	1.539805	0.180000	2.940117	1.507115	0.163231	2.958251
C	-1.710332	-0.269706	2.015375	-1.723238	-0.327834	2.028705
O	-1.556864	-0.201689	3.160518	-1.560280	-0.293286	3.172789
C	-1.669687	0.419087	-1.839801	-1.664020	0.464908	-1.827400
O	-1.449706	0.881412	-2.883339	-1.436099	0.942812	-2.861913
C	-0.136363	-1.086832	-0.077725	-0.148179	-1.095667	-0.080786
O	0.422914	-2.248453	-0.071118	0.392505	-2.259877	-0.074958
C	-2.978793	1.419106	0.310914	-2.952566	1.438604	0.365223
O	-3.481110	2.450684	0.496916	-3.444221	2.467945	0.585785
C	4.437224	-0.524094	-0.602162	4.431848	-0.511838	-0.587804
C	4.134585	-0.261551	0.758467	4.098332	-0.239001	0.763738
C	4.252812	-1.914002	-0.840676	4.282361	-1.908494	-0.812092
H	4.748547	0.205178	-1.340706	4.743227	0.214553	-1.329322
C	3.749869	-1.494837	1.366109	3.727959	-1.474186	1.378245
H	4.190245	0.697255	1.256915	4.133139	0.725232	1.253652
C	3.829647	-2.516910	0.375879	3.849626	-2.506303	0.402755
H	4.395418	-2.415256	-1.791525	4.453307	-2.417560	-1.754219
H	3.454438	-1.619460	2.401129	3.422411	-1.595077	2.410781
H	3.605088	-3.566902	0.525046	3.647797	-3.559518	0.561622
C	-0.330817	3.267592	0.891633	-0.274477	3.258305	0.928712
C	1.063751	3.197066	1.137510	1.128164	3.174504	1.129033
C	-0.528979	3.260153	-0.526556	-0.515797	3.270104	-0.482697
H	-1.106123	3.336752	1.644487	-1.024569	3.332102	1.706338
C	1.730816	3.115201	-0.118312	1.753781	3.101764	-0.147842
H	1.536874	3.194859	2.111909	1.632303	3.160112	2.087693
C	0.738345	3.169813	-1.143974	0.729927	3.176091	-1.141056
H	-1.479461	3.334943	-1.037530	-1.480665	3.359694	-0.963328
H	2.802009	3.059802	-0.269929	2.819309	3.039677	-0.333761
H	0.925100	3.117334	-2.209833	0.882491	3.136317	-2.212851
Nb	0.451032	1.085562	0.101387	0.464395	1.067054	0.100962
Nb	2.049370	-0.985843	-0.242987	2.040442	-1.012748	-0.263259
C	-4.364805	-1.192762	-0.863948	-4.374575	-1.133738	-0.900685
C	-3.398630	-2.058126	-1.460362	-3.414806	-2.004761	-1.501550
C	-4.356961	-1.436774	0.543341	-4.387804	-1.403115	0.501455
H	-5.013819	-0.504166	-1.390756	-5.006759	-0.425960	-1.422373
C	-2.803626	-2.835385	-0.431746	-2.846098	-2.811418	-0.480456
H	-3.170900	-2.127255	-2.517283	-3.177434	-2.060468	-2.557043
C	-3.388362	-2.454019	0.803367	-3.439515	-2.441644	0.754241
H	-5.000479	-0.968088	1.277671	-5.033643	-0.938209	1.236110
H	-2.015334	-3.567115	-0.561266	-2.070018	-3.555247	-0.613838
H	-3.151107	-2.876854	1.772124	-3.222682	-2.886911	1.717699
Nb	-2.247159	-0.485871	-0.027144	-2.250956	-0.469581	-0.028902

Table S26 Coordinates of $\text{Cp}_3\text{Nb}_3(\text{CO})_6$ 6-2 C_1

	BP86/SDD			BP86/LANL2DZ		
C	1.708962	0.124528	-1.890078	1.705793	0.100705	-1.903363
O	1.726887	0.610155	-2.987492	1.729042	0.581730	-3.000874
C	1.224334	0.374092	1.828675	1.218445	0.357771	1.844720
O	1.635855	0.179636	2.941063	1.624833	0.165626	2.957228
C	-1.703684	0.058085	1.926856	-1.715759	0.087792	1.923056
O	-1.625373	0.309411	3.078597	-1.644030	0.356834	3.070664
C	-1.706050	0.366294	-1.845233	-1.703094	0.377186	-1.844279
O	-1.528402	0.809669	-2.925262	-1.522057	0.821817	-2.922379
C	-0.141257	-1.113454	-0.086497	-0.150965	-1.125448	-0.083131
O	0.432177	-2.266680	-0.120018	0.407531	-2.277773	-0.121073
C	-3.099491	1.381832	0.157894	-3.098071	1.397184	0.147912
O	-3.631557	2.429468	0.260689	-3.623594	2.447783	0.246149
C	4.471951	-0.513838	-0.606108	4.469395	-0.493200	-0.593254
C	4.254383	-0.349271	0.800734	4.247830	-0.345207	0.815086
C	4.228716	-1.892002	-0.939062	4.246941	-1.872607	-0.938992
H	4.772574	0.267398	-1.309468	4.761978	0.298158	-1.288633
C	3.873942	-1.628187	1.345463	3.886193	-1.635430	1.347286
H	4.360452	0.577209	1.370128	4.344665	0.576371	1.393811
C	3.855345	-2.575212	0.267998	3.883445	-2.571930	0.261282
H	4.304887	-2.330903	-1.938001	4.331201	-2.301417	-1.941601
H	3.632440	-1.827291	2.392990	3.650840	-1.850074	2.393055
H	3.590006	-3.633706	0.350038	3.631782	-3.634568	0.333142
C	-0.324397	3.362015	0.824300	-0.291453	3.371962	0.819458
C	1.077027	3.233218	1.084489	1.109760	3.223962	1.073257
C	-0.520099	3.311239	-0.601856	-0.494528	3.319894	-0.605169
H	-1.107881	3.471661	1.579126	-1.070005	3.494473	1.577588
C	1.752442	3.085068	-0.179791	1.776978	3.064738	-0.194444
H	1.549048	3.247418	2.070342	1.586992	3.235898	2.056609
C	0.755900	3.141658	-1.219125	0.775853	3.131517	-1.228809
H	-1.477747	3.391249	-1.120854	-1.453944	3.409807	-1.119442
H	2.831106	2.995562	-0.328842	2.853947	2.966080	-0.348751
H	0.944145	3.040410	-2.291150	0.956913	3.028353	-2.301746
Nb	0.404248	1.100760	0.111789	0.408251	1.085096	0.116647
Nb	2.090447	-0.902524	-0.167695	2.086897	-0.908207	-0.167622
C	-4.395968	-1.405430	-0.745738	-4.412023	-1.397316	-0.739910
C	-3.396359	-2.261179	-1.327419	-3.418197	-2.258761	-1.323712
C	-4.326488	-1.556199	0.686576	-4.338539	-1.545923	0.692456
H	-5.102424	-0.777602	-1.294984	-5.118211	-0.767978	-1.287643
C	-2.714732	-2.936884	-0.262826	-2.736061	-2.935971	-0.260000
H	-3.194713	-2.382462	-2.395183	-3.221887	-2.383896	-2.391861
C	-3.283379	-2.504888	0.979729	-3.298516	-2.498984	0.984123
H	-4.970497	-1.062532	1.418936	-4.978650	-1.048493	1.425607
H	-1.881093	-3.634938	-0.376265	-1.905663	-3.637399	-0.374844
H	-2.983303	-2.846441	1.973924	-2.997844	-2.841356	1.977676
Nb	-2.272507	-0.522071	-0.023978	-2.278721	-0.514052	-0.024686

TableS27 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Cp}_3\text{Nb}_3(\text{CO})_9$ 9-1

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
36(0), 38(0), 38(0), 55(0), 55(0), 66(0), 66(0), 72(0), 85(1), 85(1), 87(1), 88(1), 88(1), 94(0), 101(1), 101(1), 106(0), 111(0), 116(1), 116(1), 125(1), 125(1), 127(0), 139(2), 139(2), 145(0), 157(0), 166(3), 166(3), 166(0), 298(42), 298(42), 306(1), 338(2), 338(2), 339(1), 341(4), 341(4), 343(11), 360(0), 360(0), 362(2), 407(6), 407(6), 413(46), 428(2), 430(29), 430(29), 444(57), 444(57), 446(2), 459(1), 459(1), 468(3), 468(3), 468(7), 471(9), 517(9), 533(152), 533(152), 544(12), 544(12), 544(15), 549(8), 550(27), 550(27), 612(0), 613(1), 613(1), 618(0), 618(0), 618(0), 836(136), 836(136), 836(13), 846(0), 846(0), 846(0), 849(0), 849(0), 849(0), 854(39), 854(39), 855(0), 858(5), 858(5), 859(26), 917(1), 917(0), 917(0), 941(0), 941(0), 942(0), 1031(3), 1031(3), 1031(11), 1033(5), 1033(5), 1033(3), 1081(2), 1081(2), 1081(0), 1083(0), 1083(0), 1083(0), 1150(0), 1150(0), 1150(0), 1276(0), 1276(0), 1276(0), 1425(1), 1425(1), 1425(0), 1431(0), 1431(0), 1431(7), 1472(0), 1472(0), 1472(5), 1475(0), 1475(6), 1475(6), 1931(45), 1931(45), 1978(1349), 2010(1107), 2010(1107), 2026(511), 2050(467), 2050(467), 2116(1157), 3281(1), 3281(0), 3281(0), 3286(0), 3286(0), 3286(0), 3295(0), 3295(0), 3296(2), 3298(0), 3298(0), 3298(0), 3310(0), 3310(0), 3310(0), 3310(0)	35(0), 36(0), 36(0), 53(0), 53(0), 66(0), 66(0), 71(0), 84(1), 84(1), 86(1), 87(1), 87(1), 92(0), 99(1), 99(1), 106(0), 109(0), 115(1), 115(1), 123(2), 123(2), 126(0), 137(2), 137(2), 144(0), 155(1), 163(3), 163(3), 165(0), 291(44), 291(44), 300(1), 332(1), 332(1), 333(1), 335(4), 335(4), 337(11), 356(0), 356(0), 358(2), 402(6), 402(6), 410(48), 422(3), 426(23), 426(23), 441(61), 441(61), 443(2), 455(2), 455(2), 463(2), 463(2), 463(5), 466(9), 516(8), 530(154), 530(154), 542(14), 542(22), 542(22), 547(11), 549(22), 549(22), 607(0), 607(1), 607(1), 613(0), 613(0), 613(0), 829(121), 829(121), 829(9), 841(44), 841(44), 843(1), 844(6), 844(6), 844(2), 845(10), 845(10), 846(29), 847(0), 847(3), 847(3), 904(1), 904(0), 904(0), 927(1), 927(1), 927(0), 1030(3), 1030(3), 1031(12), 1032(5), 1032(5), 1033(3), 1080(2), 1080(2), 1081(0), 1082(0), 1083(0), 1083(0), 1149(0), 1149(0), 1149(0), 1276(0), 1276(0), 1276(0), 1425(1), 1425(1), 1425(0), 1430(0), 1430(0), 1430(7), 1472(0), 1472(0), 1472(6), 1474(0), 1474(7), 1474(7), 1940(39), 1940(39), 1984(1314), 2014(1072), 2014(1072), 2031(542), 2053(466), 2053(466), 2118(1114), 3283(0), 3283(0), 3283(0), 3288(0), 3288(0), 3288(0), 3298(0), 3298(0), 3298(4), 3300(0), 3300(1), 3300(1), 3313(0), 3313(0), 3313(0), 3313(0)	26(1), 26(1), 36(0), 50(0), 50(0), 60(0), 60(0), 63(0), 77(0), 77(0), 81(1), 82(1), 82(1), 88(0), 96(2), 96(2), 98(0), 103(0), 108(1), 108(1), 118(1), 118(1), 122(0), 131(2), 131(2), 134(0), 149(0), 157(0), 162(3), 162(3), 285(44), 285(44), 290(0), 314(0), 314(0), 315(5), 319(7), 319(7), 320(7), 339(1), 339(0), 339(0), 385(4), 385(4), 392(19), 406(0), 407(31), 407(31), 426(3), 426(44), 426(44), 444(7), 444(7), 449(5), 449(5), 450(10), 451(4), 493(6), 510(108), 510(108), 510(3), 517(15), 517(15), 519(16), 521(29), 521(29), 580(0), 581(1), 581(1), 586(0), 586(0), 586(0), 798(128), 798(128), 799(17), 810(39), 810(39), 812(1), 813(1), 813(1), 813(20), 814(0), 814(0), 814(0), 817(3), 817(4), 817(4), 869(0), 869(0), 869(1), 889(0), 889(0), 889(0), 990(5), 990(5), 990(6), 992(3), 992(3), 993(7), 1042(1), 1042(1), 1042(1), 1043(0), 1043(1), 1043(1), 1104(0), 1104(0), 1104(0), 1223(0), 1223(0), 1223(0), 1361(0), 1361(0), 1361(0), 1365(0), 1365(0), 1366(6), 1408(1), 1408(1), 1408(4), 1410(4), 1410(4), 1410(0), 1813(53), 1813(53), 1857(1134), 1894(752), 1894(752), 1905(280), 1925(566), 1925(566), 1986(976), 3173(1), 3173(0), 3173(0), 3178(0), 3178(0), 3178(0), 3187(0), 3187(0), 3187(1), 3189(0), 3189(1), 3189(1), 3201(0), 3201(0), 3201(0)	23(1), 23(1), 34(0), 48(0), 48(0), 59(0), 59(0), 64(0), 77(0), 77(0), 80(1), 80(1), 80(1), 86(0), 93(1), 93(1), 97(0), 102(0), 107(1), 107(1), 116(1), 116(1), 121(0), 129(2), 129(2), 133(0), 147(0), 156(0), 159(3), 159(3), 278(45), 278(45), 285(0), 307(0), 307(0), 308(6), 313(7), 313(7), 313(7), 334(1), 335(0), 335(0), 381(4), 381(4), 389(20), 401(0), 402(27), 402(27), 424(46), 424(46), 424(3), 440(9), 440(9), 445(6), 445(6), 446(11), 447(4), 492(6), 507(111), 507(111), 508(3), 516(20), 516(20), 519(16), 522(25), 522(25), 574(0), 575(1), 575(1), 580(0), 580(0), 580(0), 791(97), 791(97), 792(13), 798(24), 798(24), 799(13), 799(55), 799(55), 801(15), 812(0), 812(0), 812(0), 814(0), 814(2), 814(2), 857(1), 857(0), 857(0), 874(1), 874(1), 875(0), 989(5), 989(5), 990(6), 992(3), 992(3), 992(9), 1041(1), 1041(1), 1041(1), 1043(0), 1043(1), 1043(1), 1103(0), 1103(0), 1103(0), 1222(0), 1223(0), 1223(0), 1360(1), 1360(1), 1361(0), 1365(0), 1365(0), 1365(6), 1408(2), 1408(2), 1408(5), 1410(4), 1410(4), 1410(1), 1822(46), 1822(46), 1864(1103), 1897(714), 1897(715), 1909(308), 1927(574), 1927(574), 1987(931), 3175(1), 3175(0), 3175(0), 3180(0), 3180(0), 3180(0), 3190(0), 3190(0), 3190(2), 3192(0), 3192(1), 3192(1), 3204(0), 3204(0), 3204(0)

Table S28 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Cp}_3\text{Nb}_3(\text{CO})_9$ 9-2

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
32(0), 43(0), 47(0), 57(0), 61(0), 64(0), 69(0), 73(0), 76(0), 82(0), 87(0), 88(0), 93(0), 99(2), 105(0), 107(2), 109(0), 114(1), 120(1), 124(0), 127(0), 134(0), 140(0), 144(0), 152(0), 154(1), 157(1), 160(0), 172(1), 200(7), 283(19), 305(36), 314(18), 327(9), 333(7), 334(4), 338(4), 339(7), 341(3), 354(2), 357(2), 362(0), 374(11), 394(35), 402(20), 410(7), 421(50), 428(19), 436(98), 437(12), 442(16), 450(18), 453(6), 466(20), 469(14), 476(31), 483(6), 502(57), 511(112), 531(33), 534(94), 537(12), 542(39), 543(12), 553(31), 567(74), 611(0), 611(1), 613(1), 616(2), 616(0), 617(0), 813(73), 826(91), 831(26), 836(12), 840(93), 843(20), 845(22), 846(1), 846(1), 847(5), 848(3), 851(0), 854(3), 857(29), 870(5), 908(0), 912(1), 919(0), 923(1), 931(0), 947(1), 1027(10), 1030(2), 1032(5), 1036(5), 1037(6), 1040(8), 1080(1), 1083(1), 1085(1), 1085(0), 1086(0), 1089(2), 1148(1), 1150(0), 1151(1), 1278(0), 1279(0), 1281(0), 1421(1), 1424(1), 1425(1), 1431(1), 1432(4), 1435(0), 1469(3), 1471(2), 1471(2), 1475(2), 1477(4), 1478(1), 1876(372), 1914(336), 1963(447), 2009(764), 2013(486), 2030(123), 2053(1004), 2079(1927), 2122(720), 3280(0), 3282(0), 3284(0), 3286(0), 3288(0), 3289(0), 3293(0), 3295(0), 3297(2), 3298(1), 3300(0), 3301(0), 3305(1), 3311(1), 3314(0)	32(0), 46(0), 50(0), 56(0), 60(0), 64(0), 69(0), 72(1), 76(0), 82(0), 86(0), 87(0), 93(0), 99(2), 103(0), 106(2), 108(0), 113(1), 117(1), 121(0), 126(0), 133(0), 139(0), 143(0), 151(0), 153(0), 156(1), 157(0), 169(1), 195(8), 277(20), 299(37), 309(18), 319(10), 327(8), 329(5), 333(3), 334(7), 336(3), 349(2), 351(2), 358(0), 372(13), 390(28), 398(22), 405(7), 418(43), 422(27), 433(3), 434(99), 438(20), 446(17), 448(7), 463(17), 465(13), 473(32), 478(5), 499(63), 508(120), 528(46), 532(74), 535(15), 540(50), 542(9), 550(28), 565(72), 605(0), 605(1), 606(2), 609(3), 610(0), 610(1), 805(57), 814(28), 818(52), 822(28), 828(51), 831(60), 833(59), 843(17), 844(6), 844(1), 845(2), 848(5), 848(21), 849(1), 858(5), 892(0), 897(0), 901(0), 911(1), 913(0), 934(1), 1026(9), 1030(3), 1030(5), 1035(4), 1037(8), 1040(6), 1081(1), 1083(1), 1084(1), 1084(0), 1085(0), 1089(2), 1147(0), 1149(0), 1150(1), 1278(0), 1279(0), 1281(0), 1421(1), 1424(1), 1425(1), 1430(1), 1431(4), 1434(0), 1468(4), 1470(2), 1471(3), 1476(3), 1477(4), 1479(1), 1889(354), 1925(340), 1967(448), 2013(744), 2017(535), 2033(114), 2057(985), 2082(1877), 2125(683), 3280(0), 3284(0), 3285(0), 3287(0), 3290(0), 3290(0), 3295(1), 3297(0), 3299(3), 3300(1), 3302(1), 3303(0), 3307(1), 3313(1), 3316(1)	32(0), 39(0), 42(0), 51(0), 53(0), 59(0), 60(0), 68(0), 72(0), 73(0), 81(0), 84(1), 86(0), 90(1), 99(0), 99(0), 100(1), 103(1), 114(1), 119(0), 123(1), 129(0), 131(0), 136(0), 143(0), 146(1), 147(0), 160(0), 196(0), 214(1), 262(2), 282(5), 291(25), 305(2), 306(9), 308(5), 313(6), 315(9), 318(1), 324(3), 333(6), 338(1), 340(0), 373(0), 385(4), 392(5), 399(24), 403(44), 410(8), 413(9), 422(71), 430(18), 431(90), 436(10), 441(85), 444(2), 466(0), 480(37), 493(61), 499(52), 507(38), 510(6), 513(60), 519(4), 527(40), 543(81), 578(0), 579(0), 580(1), 581(1), 585(0), 587(1), 760(38), 784(65), 788(67), 792(36), 796(37), 799(15), 800(94), 806(9), 813(0), 813(1), 814(5), 816(2), 818(0), 821(6), 822(1), 857(0), 863(1), 868(0), 873(1), 873(0), 891(2), 984(7), 990(3), 992(5), 994(4), 996(2), 998(12), 1039(1), 1043(0), 1045(0), 1045(1), 1046(1), 1050(2), 1103(1), 1103(0), 1105(2), 1225(0), 1226(0), 1227(0), 1357(1), 1360(1), 1361(1), 1365(3), 1366(0), 1371(0), 1404(2), 1408(1), 1409(2), 1410(4), 1412(1), 1414(2), 1743(339), 1771(220), 1861(325), 1892(768), 1895(45), 1913(119), 1930(785), 1947(1681), 1990(728), 3173(0), 3174(0), 3176(0), 3178(0), 3179(0), 3181(0), 3186(0), 3186(1), 3190(1), 3190(0), 3191(0), 3192(0), 3196(1), 3200(1), 3204(0)	32(0), 37(0), 37(0), 50(0), 53(0), 57(0), 59(0), 68(0), 71(0), 73(0), 81(0), 83(1), 85(0), 89(1), 98(1), 98(1), 99(0), 102(1), 111(1), 117(0), 122(1), 129(0), 130(0), 134(0), 141(0), 146(1), 146(0), 158(0), 192(0), 212(1), 256(3), 273(5), 285(23), 299(10), 300(4), 302(4), 307(6), 310(10), 312(1), 319(4), 326(7), 333(1), 336(0), 368(0), 381(5), 390(7), 396(20), 400(45), 406(6), 410(11), 419(60), 424(15), 428(99), 433(6), 438(87), 440(11), 462(0), 477(38), 490(60), 497(65), 505(38), 509(8), 512(60), 517(3), 527(37), 542(73), 571(0), 573(0), 575(1), 575(1), 579(0), 581(2), 747(25), 769(2), 775(73), 778(32), 786(55), 786(78), 794(37), 795(70), 809(6), 811(1), 811(1), 812(4), 814(1), 815(0), 818(1), 842(0), 847(1), 854(0), 858(1), 861(0), 877(1), 983(7), 989(3), 990(5), 993(4), 995(3), 997(12), 1038(1), 1043(0), 1044(0), 1045(1), 1045(1), 1049(3), 1102(0), 1102(0), 1104(1), 1224(0), 1225(0), 1226(0), 1356(1), 1360(1), 1360(1), 1364(3), 1366(1), 1370(0), 1403(3), 1407(2), 1408(2), 1410(4), 1412(1), 1414(2), 1754(324), 1781(213), 1865(329), 1896(765), 1897(62), 1916(109), 1934(771), 1950(1634), 1993(692), 3174(0), 3176(0), 3178(0), 3179(0), 3180(0), 3183(0), 3188(0), 3188(0), 3192(0), 3192(1), 3193(0), 3194(0), 3199(1), 3203(1), 3206(0)

Table S29 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Cp}_3\text{Nb}_3(\text{CO})_9$ 9-3

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
26(1), 41(2), 49(0), 54(1), 63(0), 67(0), 74(0), 75(0), 80(0), 85(0), 88(0), 92(0), 99(0), 100(0), 104(0), 106(0), 110(0), 116(0), 117(1), 121(1), 124(0), 134(1), 143(1), 148(1), 154(1), 157(3), 164(2), 174(3), 186(3), 190(0), 290(6), 302(12), 312(33), 321(27), 327(5), 329(12), 333(3), 336(5), 341(11), 351(2), 356(3), 368(23), 372(1), 384(26), 403(9), 424(15), 425(25), 429(31), 440(8), 445(45), 450(13), 455(36), 459(19), 462(17), 469(57), 472(2), 481(2), 503(32), 507(137), 526(45), 538(11), 544(82), 549(43), 550(37), 561(8), 570(18), 610(0), 611(0), 614(1), 615(1), 616(1), 618(0), 803(53), 823(94), 832(33), 837(26), 839(125), 841(26), 845(13), 846(6), 847(5), 849(4), 850(0), 850(2), 852(30), 854(3), 865(13), 906(1), 912(1), 918(0), 921(2), 926(0), 942(0), 1027(9), 1030(3), 1031(2), 1036(2), 1037(4), 1040(10), 1077(1), 1083(0), 1084(1), 1084(0), 1086(0), 1090(1), 1150(0), 1150(0), 1152(1), 1276(0), 1278(0), 1279(0), 1424(1), 1424(2), 1425(3), 1428(1), 1431(1), 1435(0), 1469(2), 1470(5), 1472(2), 1475(1), 1475(2), 1479(3), 1886(396), 1926(713), 1946(382), 1968(176), 2001(862), 2037(45), 2060(1737), 2068(988), 2117(1691), 3279(0), 3282(0), 3285(0), 3286(0), 3286(0), 3295(2), 3295(1), 3296(0), 3298(0), 3299(0), 3302(1), 3309(1), 3311(1), 3312(1), 3324(0)	29(1), 39(2), 49(0), 52(0), 63(0), 65(0), 71(0), 72(0), 79(0), 85(0), 87(0), 91(0), 98(0), 100(0), 103(0), 105(0), 109(0), 115(0), 116(1), 120(1), 122(0), 132(1), 142(1), 146(1), 152(2), 155(3), 163(1), 176(3), 184(3), 189(0), 286(9), 296(10), 307(31), 314(29), 320(7), 324(7), 327(6), 330(5), 336(10), 347(2), 351(3), 365(19), 368(2), 381(25), 400(8), 420(18), 422(21), 426(32), 436(9), 442(35), 446(20), 451(41), 455(17), 460(18), 465(57), 468(4), 476(4), 501(27), 506(153), 522(47), 537(32), 543(61), 548(41), 549(32), 559(10), 570(21), 605(0), 606(0), 609(0), 610(1), 610(1), 612(0), 795(40), 812(50), 821(60), 823(26), 827(42), 833(83), 835(88), 843(15), 844(4), 845(10), 847(3), 848(6), 848(1), 850(2), 857(13), 892(1), 898(1), 902(0), 913(2), 913(0), 934(0), 1026(9), 1030(3), 1030(3), 1035(2), 1037(4), 1039(10), 1076(2), 1083(1), 1083(1), 1084(0), 1087(1), 1088(1), 1149(0), 1150(0), 1152(1), 1275(0), 1278(0), 1278(0), 1424(1), 1424(2), 1425(4), 1427(1), 1431(1), 1434(0), 1469(1), 1470(6), 1472(2), 1475(2), 1476(3), 1479(3), 1898(384), 1930(557), 1946(427), 1977(259), 2005(835), 2042(38), 2063(1689), 2072(1014), 2120(1665), 3280(0), 3283(0), 3286(0), 3287(0), 3287(0), 3296(2), 3297(1), 3298(1), 3301(0), 3302(0), 3304(1), 3311(1), 3312(1), 3316(1), 3325(1)	23(0), 32(0), 46(0), 49(0), 51(0), 64(0), 71(0), 73(0), 75(0), 81(0), 85(0), 86(0), 91(0), 94(0), 97(0), 100(1), 105(0), 107(0), 110(0), 113(0), 125(0), 126(1), 136(1), 149(1), 152(0), 156(0), 162(1), 178(0), 189(1), 208(0), 267(3), 276(2), 284(9), 297(7), 301(11), 304(19), 307(4), 312(8), 315(7), 328(5), 331(5), 336(0), 357(7), 365(16), 374(6), 393(24), 400(11), 404(9), 416(79), 418(12), 422(62), 431(32), 435(17), 438(19), 446(44), 459(1), 462(6), 474(36), 478(48), 496(60), 510(50), 513(60), 520(42), 526(16), 532(32), 541(14), 577(1), 577(0), 578(1), 581(0), 582(1), 585(1), 767(48), 781(37), 786(42), 791(91), 800(23), 800(124), 804(10), 808(31), 814(2), 814(1), 816(5), 818(4), 818(2), 820(1), 824(7), 857(3), 861(0), 869(1), 876(0), 879(6), 888(2), 986(8), 989(1), 990(3), 994(3), 1001(10), 1002(3), 1040(1), 1041(1), 1045(0), 1045(1), 1046(0), 1056(1), 1103(1), 1105(0), 1106(2), 1223(0), 1227(0), 1228(0), 1357(1), 1357(3), 1360(2), 1362(1), 1368(0), 1371(0), 1405(3), 1406(2), 1407(2), 1409(1), 1415(1), 1416(2), 1687(348), 1798(316), 1841(454), 1875(552), 1881(82), 1919(35), 1940(1608), 1944(661), 1989(1462), 3172(0), 3174(0), 3176(0), 3176(0), 3179(0), 3186(0), 3187(0), 3188(1), 3188(0), 3188(0), 3195(0), 3198(1), 3199(1), 3202(0), 3213(0)	21(0), 33(0), 44(0), 49(0), 50(0), 62(0), 69(0), 72(0), 75(0), 79(0), 84(0), 84(0), 90(0), 92(0), 96(0), 99(1), 103(0), 107(0), 109(0), 111(1), 122(0), 125(1), 134(1), 149(1), 151(0), 155(0), 160(1), 177(0), 186(1), 206(0), 260(4), 271(2), 276(8), 290(6), 295(11), 298(21), 300(3), 306(7), 309(8), 322(5), 326(5), 331(1), 355(8), 363(11), 371(8), 388(19), 397(10), 401(10), 414(86), 415(10), 420(45), 428(44), 431(18), 436(21), 442(47), 456(1), 461(6), 472(34), 477(51), 493(58), 507(54), 510(60), 518(44), 525(17), 531(30), 542(15), 571(0), 572(1), 574(1), 575(0), 576(1), 579(1), 754(30), 767(17), 769(37), 780(101), 785(21), 794(91), 796(72), 797(47), 811(6), 812(5), 812(1), 815(1), 816(4), 817(1), 818(1), 840(3), 847(1), 850(1), 862(0), 871(6), 880(2), 984(9), 988(1), 990(3), 994(3), 1001(11), 1002(3), 1039(1), 1041(1), 1045(0), 1045(1), 1045(0), 1056(2), 1103(0), 1105(0), 1106(1), 1223(0), 1226(0), 1227(0), 1357(1), 1357(4), 1359(2), 1361(1), 1367(1), 1370(0), 1404(4), 1406(2), 1407(2), 1409(2), 1415(1), 1416(3), 1700(335), 1807(306), 1847(440), 1878(529), 1882(90), 1922(57), 1942(1526), 1946(694), 1992(1429), 3173(0), 3176(0), 3178(0), 3178(0), 3180(0), 3189(0), 3189(1), 3190(0), 3191(0), 3191(0), 3196(0), 3201(1), 3203(1), 3205(1), 3216(1)

Table S30 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Cp}_3\text{Nb}_3(\text{CO})_9$, 9-4

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
20(0), 27(0), 39(1), 49(0), 53(1), 57(0), 61(0), 64(1), 71(1), 76(0), 78(1), 85(0), 88(0), 92(1), 96(1), 101(2), 102(0), 106(1), 112(0), 113(1), 122(1), 127(1), 135(3), 143(2), 150(1), 154(0), 180(4), 184(0), 230(3), 265(11), 301(34), 306(31), 319(3), 322(4), 331(1), 332(8), 337(4), 343(1), 347(8), 347(4), 356(11), 358(7), 366(0), 392(26), 400(12), 407(6), 415(5), 418(9), 426(8), 429(63), 435(33), 439(14), 446(7), 451(2), 456(13), 462(15), 472(1), 491(61), 506(9), 523(57), 526(16), 535(45), 542(4), 545(40), 568(140), 610(0), 613(0), 614(0), 617(0), 619(0), 622(0), 700(144), 806(51), 821(75), 835(89), 839(4), 841(5), 844(42), 845(23), 846(9), 846(16), 846(14), 849(20), 850(4), 851(6), 858(6), 862(11), 904(0), 906(1), 915(1), 933(1), 939(3), 942(3), 1014(8), 1030(9), 1031(4), 1035(7), 1037(4), 1042(13), 1075(0), 1081(0), 1083(1), 1084(1), 1085(2), 1085(1), 1145(0), 1149(1), 1153(1), 1274(0), 1278(0), 1278(0), 1419(6), 1421(1), 1422(8), 1428(1), 1429(1), 1432(2), 1468(1), 1471(4), 1472(3), 1475(2), 1479(2), 1484(2), 1566(141), 1807(371), 1919(566), 2001(612), 2031(494), 2032(499), 2073(455), 2090(1976), 2124(417), 3279(0), 3280(0), 3280(0), 3281(0), 3284(0), 3287(0), 3292(2), 3293(0), 3294(0), 3295(0), 3297(0), 3298(1), 3303(0), 3309(0), 3309(1)	14(0), 25(0), 38(1), 48(0), 52(1), 55(0), 60(0), 63(1), 70(1), 75(0), 77(1), 84(0), 87(0), 90(1), 94(1), 99(3), 100(0), 105(1), 110(0), 112(0), 120(1), 125(1), 134(3), 141(2), 148(1), 152(0), 177(3), 181(0), 229(4), 262(10), 297(31), 300(35), 314(2), 319(4), 325(2), 327(7), 331(4), 337(1), 342(10), 344(3), 351(14), 354(5), 363(0), 389(26), 398(10), 404(6), 410(6), 414(9), 422(5), 425(55), 431(42), 434(16), 442(5), 446(2), 452(16), 457(17), 469(3), 489(60), 504(9), 521(57), 523(16), 535(42), 542(8), 545(46), 566(145), 604(0), 607(0), 609(0), 611(0), 613(0), 616(0), 695(157), 797(50), 811(56), 821(5), 825(63), 832(52), 834(54), 838(23), 840(54), 843(0), 844(2), 847(3), 847(1), 847(2), 849(10), 850(8), 890(0), 894(0), 902(1), 912(1), 930(3), 931(3), 1013(8), 1029(9), 1030(4), 1034(7), 1037(5), 1041(12), 1075(0), 1081(0), 1082(1), 1083(1), 1084(1), 1084(2), 1145(0), 1148(0), 1152(0), 1274(0), 1277(0), 1278(0), 1419(6), 1421(1), 1422(8), 1428(1), 1429(1), 1431(2), 1468(1), 1471(4), 1471(3), 1475(3), 1479(2), 1484(2), 1581(143), 1822(364), 1932(555), 2007(589), 2035(474), 2037(503), 2077(451), 2093(1968), 2127(364), 3280(0), 3281(0), 3282(0), 3283(0), 3284(0), 3289(0), 3293(2), 3295(0), 3296(0), 3298(0), 3298(1), 3301(1), 3306(0), 3311(1), 3311(0)	30(0), 33(0), 43(0), 50(0), 54(1), 56(1), 59(1), 62(0), 69(1), 75(0), 75(0), 81(0), 83(0), 91(1), 93(1), 96(1), 99(0), 101(0), 108(2), 110(1), 117(0), 124(0), 128(1), 132(2), 140(2), 148(0), 175(0), 198(4), 228(1), 255(12), 280(34), 287(15), 304(5), 306(1), 311(2), 314(4), 315(3), 321(0), 327(16), 332(2), 337(3), 341(8), 346(2), 364(23), 379(13), 385(10), 391(4), 397(5), 403(8), 410(79), 416(18), 419(22), 428(4), 430(15), 434(3), 441(5), 448(1), 465(28), 473(55), 495(20), 499(23), 510(27), 512(22), 521(14), 546(119), 576(0), 580(1), 582(0), 585(0), 586(0), 589(0), 633(117), 768(37), 783(79), 793(5), 799(97), 799(27), 802(72), 805(26), 807(0), 814(2), 814(2), 815(3), 815(4), 818(0), 818(0), 821(15), 856(0), 856(1), 869(1), 880(1), 885(4), 892(2), 973(7), 989(8), 990(4), 996(7), 998(4), 1000(12), 1036(0), 1042(0), 1043(1), 1044(1), 1045(3), 1047(0), 1098(1), 1103(1), 1108(0), 1222(0), 1225(0), 1226(0), 1354(7), 1356(5), 1358(1), 1363(1), 1366(1), 1369(1), 1401(0), 1408(2), 1409(3), 1412(2), 1415(2), 1418(2), 1481(133), 1708(260), 1777(439), 1880(363), 1901(352), 1907(600), 1940(465), 1959(1661), 1988(350), 3171(0), 3171(0), 3172(0), 3173(0), 3176(0), 3178(0), 3184(0), 3184(1), 3185(0), 3186(1), 3188(0), 3190(0), 3194(0), 3199(0), 3200(0)	30(0), 33(0), 42(1), 47(0), 52(1), 54(1), 58(1), 60(0), 68(1), 73(0), 75(0), 79(0), 82(0), 90(1), 92(1), 94(1), 98(0), 100(0), 106(1), 109(0), 116(0), 122(1), 126(1), 130(3), 138(2), 146(0), 172(0), 195(4), 228(2), 252(10), 274(34), 279(16), 299(5), 301(1), 307(4), 309(1), 310(3), 315(1), 323(18), 327(2), 332(3), 337(7), 342(2), 362(24), 376(12), 382(10), 387(4), 393(5), 398(7), 407(80), 412(17), 415(27), 422(5), 427(14), 431(5), 439(7), 444(1), 463(27), 470(54), 494(20), 497(24), 511(17), 513(33), 520(16), 544(124), 570(0), 575(1), 576(0), 579(1), 580(0), 584(0), 628(127), 758(33), 774(47), 776(6), 786(64), 788(35), 794(93), 796(69), 803(1), 805(3), 808(14), 812(2), 812(2), 813(2), 815(0), 816(1), 842(1), 846(0), 857(1), 860(1), 876(3), 878(2), 972(7), 989(9), 989(4), 995(7), 997(4), 999(12), 1036(0), 1042(0), 1042(1), 1044(1), 1044(3), 1046(0), 1097(0), 1102(1), 1107(0), 1221(0), 1224(0), 1225(0), 1355(7), 1355(6), 1358(1), 1363(1), 1365(1), 1368(1), 1400(1), 1407(2), 1409(3), 1412(3), 1415(2), 1418(2), 1495(134), 1720(251), 1788(427), 1884(341), 1905(359), 1911(578), 1943(466), 1961(1643), 1991(308), 3172(0), 3173(0), 3173(0), 3175(0), 3177(0), 3180(0), 3186(1), 3187(0), 3188(0), 3189(1), 3190(0), 3193(0), 3198(0), 3202(0), 3202(1)

Table S31 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Cp}_3\text{Nb}_3(\text{CO})_8$ 8-1

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
28(0), 35(0), 49(0), 61(1), 66(1), 72(0), 74(0), 78(0), 86(0), 91(0), 94(1), 94(0), 96(1), 100(1), 101(0), 108(2), 111(1), 116(0), 119(1), 123(2), 133(1), 145(2), 145(2), 155(3), 157(1), 162(1), 185(1), 220(1), 305(32), 315(3), 322(3), 324(2), 336(4), 340(3), 342(2), 345(4), 356(0), 359(5), 383(25), 393(15), 408(16), 425(27), 430(41), 438(46), 444(65), 447(11), 455(4), 460(4), 463(7), 469(0), 483(7), 494(12), 511(21), 518(30), 528(79), 539(37), 547(5), 550(6), 560(21), 572(17), 583(74), 610(4), 612(1), 614(1), 614(1), 617(0), 619(2), 812(59), 825(87), 835(104), 837(60), 844(2), 846(1), 847(5), 848(1), 848(2), 850(4), 852(9), 852(5), 852(10), 857(18), 862(45), 910(0), 914(1), 916(0), 932(4), 939(0), 943(1), 1029(4), 1033(5), 1033(6), 1034(6), 1035(4), 1043(9), 1081(1), 1082(1), 1084(2), 1085(0), 1086(2), 1087(6), 1151(0), 1152(0), 1152(0), 1278(0), 1279(0), 1280(0), 1420(1), 1425(1), 1426(1), 1427(2), 1430(4), 1436(3), 1470(4), 1471(4), 1473(2), 1474(4), 1481(2), 1482(4), 1783(223), 1943(55), 1960(360), 1999(1118), 2008(1056), 2021(1376), 2050(1318), 2089(387), 3279(0), 3281(0), 3282(0), 3286(0), 3287(0), 3287(0), 3295(1), 3295(1), 3296(1), 3298(0), 3300(0), 3302(0), 3314(0), 3315(0), 3317(0)	29(0), 33(0), 49(0), 60(1), 64(0), 70(0), 74(0), 77(0), 84(0), 89(0), 92(3), 94(0), 96(0), 98(0), 100(1), 106(1), 111(0), 113(0), 119(1), 123(2), 130(1), 144(2), 144(1), 153(3), 155(1), 160(1), 179(0), 211(1), 299(34), 311(3), 315(4), 319(1), 330(4), 334(3), 336(2), 339(4), 351(0), 356(6), 382(24), 387(14), 405(20), 422(15), 429(33), 436(62), 441(60), 445(10), 452(3), 456(5), 458(14), 465(0), 478(7), 492(11), 508(29), 514(23), 526(83), 539(33), 548(1), 549(9), 560(40), 573(15), 578(66), 604(4), 607(0), 607(1), 609(1), 612(0), 615(2), 805(37), 815(82), 828(87), 831(76), 831(33), 840(2), 841(16), 843(5), 843(31), 844(3), 846(3), 846(10), 847(4), 849(33), 849(1), 900(1), 900(0), 904(0), 922(5), 925(1), 927(0), 1027(4), 1032(4), 1032(7), 1033(6), 1034(4), 1041(10), 1080(1), 1082(2), 1082(7), 1084(0), 1084(2), 1085(1), 1151(0), 1151(0), 1152(0), 1277(0), 1277(0), 1279(0), 1420(2), 1425(2), 1426(0), 1427(2), 1430(4), 1435(3), 1469(5), 1471(4), 1473(3), 1474(4), 1481(2), 1483(4), 1802(233), 1950(63), 1967(291), 2004(1017), 2012(1176), 2026(1334), 2053(1238), 2092(384), 3280(0), 3283(0), 3284(0), 3287(0), 3288(0), 3289(0), 3297(1), 3297(1), 3298(1), 3301(0), 3302(0), 3303(0), 3316(0), 3317(0), 3318(0)	25(0), 30(0), 40(0), 57(1), 60(1), 66(0), 68(0), 72(0), 81(1), 85(0), 87(0), 87(0), 90(1), 94(0), 96(0), 101(1), 104(1), 107(1), 111(0), 115(2), 125(1), 136(1), 137(1), 147(2), 152(2), 158(1), 178(1), 211(1), 292(27), 294(3), 299(5), 303(3), 313(4), 317(8), 320(1), 321(4), 333(0), 338(3), 366(16), 375(9), 386(7), 406(24), 408(26), 421(57), 425(40), 430(2), 440(12), 441(12), 445(7), 452(1), 459(7), 474(7), 487(9), 496(22), 506(65), 513(21), 517(6), 523(6), 529(15), 541(11), 552(67), 579(5), 580(0), 581(1), 582(1), 586(0), 587(1), 777(49), 787(80), 794(74), 797(98), 804(17), 805(3), 809(16), 810(10), 812(3), 815(0), 816(3), 816(5), 817(2), 819(0), 822(39), 863(0), 867(2), 868(0), 882(3), 884(0), 892(1), 988(3), 991(4), 992(7), 994(4), 994(5), 1003(9), 1041(1), 1043(1), 1045(1), 1045(4), 1046(5), 1046(1), 1105(0), 1105(0), 1106(0), 1225(0), 1226(0), 1227(0), 1355(1), 1360(2), 1362(1), 1363(1), 1365(3), 1371(2), 1406(4), 1407(4), 1409(3), 1411(2), 1416(2), 1418(4), 1682(161), 1828(55), 1844(328), 1881(837), 1890(798), 1901(1074), 1927(1334), 1957(256), 3171(0), 3172(0), 3175(0), 3178(0), 3178(0), 3179(0), 3187(1), 3187(1), 3187(0), 3190(0), 3192(0), 3194(0), 3204(0), 3207(0), 3207(0)	30(0), 31(0), 43(0), 56(1), 59(0), 66(0), 68(0), 70(0), 79(1), 83(0), 85(0), 87(1), 89(0), 93(1), 94(0), 99(1), 104(1), 105(1), 110(1), 115(2), 123(1), 135(2), 136(1), 144(1), 150(3), 153(1), 172(0), 203(1), 285(26), 290(4), 291(7), 297(1), 306(4), 310(11), 314(1), 315(4), 327(0), 335(4), 365(14), 370(8), 384(8), 405(28), 406(11), 417(46), 420(50), 428(2), 436(19), 438(20), 442(5), 449(1), 455(7), 472(7), 484(11), 492(23), 504(68), 511(17), 516(0), 522(6), 529(35), 540(17), 548(50), 572(4), 575(0), 575(1), 576(1), 580(0), 582(1), 756(32), 777(67), 786(23), 789(73), 791(67), 794(10), 798(47), 799(41), 806(44), 810(0), 812(0), 813(1), 814(0), 815(2), 816(0), 850(1), 853(1), 855(0), 873(0), 874(4), 874(1), 986(4), 990(4), 992(8), 993(6), 994(4), 1000(9), 1041(1), 1041(3), 1042(6), 1044(1), 1045(1), 1046(1), 1104(0), 1105(0), 1105(0), 1224(0), 1225(0), 1226(0), 1355(2), 1360(2), 1361(1), 1362(1), 1364(3), 1370(2), 1404(5), 1407(4), 1408(3), 1410(2), 1416(2), 1419(4), 1699(165), 1833(66), 1850(291), 1885(762), 1894(857), 1905(1023), 1930(1272), 1959(263), 3171(0), 3174(0), 3176(0), 3180(0), 3180(0), 3181(0), 3189(1), 3189(1), 3191(1), 3193(0), 3194(0), 3195(0), 3206(0), 3208(0), 3209(0)

Table S32 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Cp}_3\text{Nb}_3(\text{CO})_8$ 8-2

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
18(0), 36(0), 39(1), 46(0), 47(0), 63(0), 69(1), 74(0), 78(0), 86(0), 88(0), 93(2), 96(2), 99(0), 104(0), 106(0), 109(1), 120(0), 125(1), 130(1), 134(1), 142(1), 151(3), 158(0), 164(0), 177(1), 240(1), 288(1), 297(2), 305(2), 312(9), 324(5), 325(2), 332(3), 341(4), 346(2), 357(4), 381(7), 385(44), 396(6), 401(22), 411(55), 429(20), 439(14), 443(34), 445(42), 449(1), 457(17), 462(33), 466(15), 477(7), 482(4), 490(17), 499(6), 513(17), 525(39), 542(14), 563(10), 571(8), 584(44), 609(3), 612(6), 613(0), 616(1), 617(1), 620(1), 631(38), 802(51), 820(89), 826(104), 830(76), 835(27), 839(12), 842(12), 845(19), 849(7), 849(9), 850(1), 850(3), 852(8), 855(21), 856(25), 906(0), 910(2), 920(4), 930(1), 933(3), 946(4), 1027(5), 1028(5), 1028(6), 1035(4), 1036(7), 1039(3), 1079(0), 1081(3), 1081(1), 1082(2), 1084(0), 1089(1), 1147(2), 1149(0), 1151(0), 1276(0), 1278(0), 1280(0), 1417(0), 1417(2), 1420(4), 1427(3), 1428(1), 1429(3), 1470(2), 1471(1), 1474(5), 1476(7), 1476(1), 1481(1), 1517(132), 1905(182), 1998(725), 2011(570), 2024(526), 2058(1047), 2062(1942), 2102(945), 3277(0), 3279(0), 3281(0), 3284(0), 3287(0), 3288(0), 3293(1), 3297(0), 3298(0), 3300(0), 3300(0), 3304(1), 3313(0), 3316(1), 3322(0)	19(0), 35(0), 37(1), 44(0), 48(0), 63(0), 68(1), 73(0), 77(0), 84(0), 87(0), 94(2), 95(2), 98(0), 104(0), 106(0), 110(1), 121(0), 126(1), 129(1), 133(1), 142(1), 151(3), 159(0), 163(1), 177(1), 236(1), 280(1), 291(2), 298(2), 305(8), 318(6), 320(1), 326(3), 334(6), 341(2), 352(3), 378(7), 380(45), 392(5), 400(25), 409(49), 426(18), 436(24), 440(20), 442(50), 446(2), 455(18), 459(39), 464(13), 475(4), 481(3), 488(19), 498(7), 513(18), 524(39), 541(17), 561(12), 571(6), 584(46), 604(3), 607(5), 608(1), 612(2), 612(0), 615(1), 628(40), 798(41), 810(62), 820(110), 822(53), 825(69), 831(15), 833(15), 839(41), 845(20), 845(30), 847(2), 848(0), 849(0), 850(11), 852(10), 895(1), 902(2), 909(4), 918(1), 923(4), 934(3), 1027(5), 1027(2), 1027(9), 1035(4), 1037(7), 1039(3), 1079(0), 1080(3), 1081(1), 1082(2), 1084(1), 1089(1), 1148(1), 1150(0), 1152(1), 1276(0), 1277(0), 1279(0), 1418(0), 1418(2), 1420(4), 1427(1), 1428(2), 1429(3), 1470(2), 1472(2), 1474(6), 1477(7), 1477(1), 1482(1), 1539(137), 1907(185), 2000(722), 2016(560), 2028(542), 2062(1128), 2066(1701), 2105(977), 3277(0), 3279(0), 3281(0), 3285(0), 3287(0), 3288(0), 3294(1), 3299(1), 3299(0), 3301(0), 3301(0), 3306(1), 3314(1), 3319(1), 3325(1)	22(0), 33(0), 37(0), 41(0), 54(0), 61(0), 66(0), 73(1), 75(0), 82(0), 84(0), 88(0), 91(2), 95(1), 101(0), 104(0), 105(1), 116(0), 121(1), 124(1), 129(1), 138(1), 142(2), 152(0), 156(1), 171(0), 226(1), 268(2), 277(3), 283(2), 296(8), 301(5), 304(1), 310(3), 319(4), 325(4), 335(1), 364(5), 370(23), 380(5), 382(15), 405(70), 411(10), 419(2), 424(26), 428(15), 432(9), 437(49), 446(20), 448(15), 457(2), 465(3), 470(10), 476(5), 490(13), 498(28), 515(12), 533(8), 542(7), 550(35), 577(17), 580(1), 581(1), 583(2), 584(0), 586(0), 590(20), 764(40), 782(72), 786(47), 790(77), 791(76), 798(6), 804(18), 805(49), 812(3), 814(44), 817(1), 818(1), 818(2), 819(3), 821(5), 855(0), 867(4), 869(2), 880(4), 882(2), 899(3), 987(1), 987(9), 989(5), 995(4), 995(5), 1000(3), 1041(3), 1041(0), 1042(1), 1044(2), 1046(0), 1050(1), 1101(2), 1103(0), 1105(0), 1225(0), 1225(0), 1227(0), 1353(0), 1353(2), 1356(4), 1362(1), 1363(1), 1365(2), 1406(2), 1408(1), 1409(5), 1411(6), 1412(1), 1416(1), 1443(104), 1794(123), 1878(529), 1894(492), 1904(341), 1931(854), 1936(1916), 1971(744), 3169(0), 3170(0), 3174(0), 3176(0), 3178(0), 3180(0), 3185(0), 3189(0), 3189(0), 3191(0), 3192(0), 3195(1), 3203(0), 3206(0), 3217(1)	25(0), 30(0), 38(0), 42(0), 53(0), 63(0), 66(1), 74(1), 76(0), 81(0), 83(0), 89(0), 90(2), 94(1), 100(0), 103(0), 104(2), 115(0), 120(1), 123(1), 127(1), 137(1), 141(3), 152(0), 155(0), 169(0), 222(1), 259(1), 270(4), 275(3), 287(8), 295(4), 298(2), 303(4), 309(5), 320(3), 330(1), 362(5), 367(22), 377(3), 380(17), 403(69), 408(12), 418(2), 421(34), 425(4), 429(11), 435(56), 444(20), 447(12), 455(2), 464(6), 468(8), 475(6), 490(13), 497(27), 515(13), 533(10), 542(5), 551(36), 571(5), 573(10), 576(2), 577(1), 580(0), 581(0), 586(23), 757(26), 772(53), 779(34), 783(85), 784(96), 786(7), 795(22), 799(65), 806(57), 809(3), 815(0), 815(0), 816(1), 817(1), 819(5), 847(1), 857(3), 859(4), 870(4), 871(3), 888(3), 986(1), 987(9), 989(5), 995(4), 996(6), 999(3), 1041(1), 1041(4), 1042(1), 1044(2), 1046(0), 1049(1), 1102(1), 1104(0), 1105(1), 1225(0), 1225(0), 1227(0), 1352(0), 1354(2), 1356(4), 1362(1), 1364(1), 1365(2), 1406(2), 1409(2), 1409(6), 1411(5), 1412(1), 1417(1), 1463(105), 1798(120), 1880(518), 1897(478), 1908(340), 1934(822), 1939(1856), 1973(738), 3169(0), 3171(0), 3174(0), 3178(0), 3178(0), 3181(0), 3187(1), 3190(0), 3191(0), 3192(0), 3194(0), 3197(1), 3205(0), 3210(0), 3218(1)

Table S33 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Cp}_3\text{Nb}_3(\text{CO})_8$ 8-3

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
21(1), 37(0), 41(0), 55(1), 59(0), 65(0), 73(0), 76(1), 78(1), 84(0), 88(0), 93(1), 95(0), 98(0), 103(0), 104(0), 106(1), 112(2), 118(1), 125(1), 132(0), 144(1), 150(2), 159(1), 167(1), 182(0), 217(3), 232(1), 310(21), 321(20), 325(1), 329(6), 332(5), 335(6), 339(2), 343(9), 347(3), 357(1), 358(12), 365(23), 388(21), 398(13), 404(18), 413(38), 416(27), 429(4), 441(9), 444(20), 452(9), 457(4), 464(14), 468(24), 482(13), 490(9), 503(56), 527(25), 532(46), 544(5), 552(12), 562(14), 587(85), 609(1), 614(1), 615(0), 615(1), 619(0), 620(0), 827(101), 830(28), 831(82), 836(112), 846(2), 846(6), 847(17), 848(4), 849(10), 850(5), 851(6), 852(5), 853(7), 859(10), 867(24), 921(2), 922(3), 928(1), 931(7), 938(0), 942(0), 1028(10), 1032(5), 1033(7), 1037(4), 1037(4), 1039(8), 1081(1), 1082(2), 1084(0), 1085(0), 1085(0), 1087(0), 1151(2), 1152(0), 1154(0), 1278(0), 1278(0), 1279(0), 1423(2), 1426(0), 1427(0), 1432(2), 1432(3), 1437(1), 1469(1), 1472(3), 1473(5), 1476(1), 1479(5), 1485(2), 1837(695), 1859(818), 1955(293), 1966(360), 2022(1065), 2034(724), 2056(607), 2105(1210), 3279(0), 3280(0), 3281(1), 3285(0), 3285(0), 3291(0), 3291(1), 3295(0), 3297(1), 3300(0), 3300(0), 3302(2), 3303(0), 3311(0), 3312(1)	21(1), 39(0), 42(1), 54(1), 58(0), 65(0), 71(0), 75(0), 77(1), 84(1), 87(0), 93(0), 93(0), 97(0), 102(0), 103(0), 105(1), 109(2), 117(1), 124(1), 129(0), 143(0), 148(2), 157(1), 165(1), 180(0), 212(2), 232(1), 307(23), 315(11), 317(5), 322(7), 325(7), 329(5), 334(2), 339(9), 342(3), 353(1), 354(10), 362(22), 384(23), 394(15), 401(18), 411(40), 414(25), 426(4), 438(9), 440(18), 448(9), 452(3), 460(13), 464(23), 477(17), 489(9), 501(58), 526(34), 532(50), 544(6), 552(13), 561(14), 587(92), 603(1), 609(2), 609(0), 610(2), 613(0), 614(0), 808(3), 815(93), 822(81), 831(128), 834(15), 835(39), 840(7), 843(5), 845(2), 845(4), 847(0), 848(5), 849(0), 851(4), 853(36), 907(5), 907(4), 909(2), 910(1), 923(0), 925(0), 1028(10), 1031(5), 1032(7), 1036(3), 1036(6), 1038(8), 1080(1), 1081(2), 1083(0), 1084(1), 1085(0), 1086(0), 1151(1), 1151(0), 1153(0), 1277(0), 1277(0), 1279(0), 1423(2), 1426(1), 1427(0), 1431(3), 1432(3), 1436(1), 1469(1), 1472(4), 1473(5), 1476(2), 1479(5), 1485(3), 1850(725), 1872(764), 1959(136), 1965(528), 2027(1019), 2041(712), 2062(583), 2108(1175), 3280(0), 3281(0), 3282(1), 3287(0), 3287(0), 3292(1), 3293(1), 3297(0), 3299(1), 3302(1), 3303(0), 3305(3), 3305(0), 3314(1), 3315(1)	21(1), 26(0), 33(0), 50(0), 54(0), 58(1), 67(0), 69(0), 72(1), 78(1), 79(0), 84(1), 92(0), 93(0), 97(0), 101(1), 101(0), 109(1), 111(0), 118(1), 128(0), 134(0), 139(2), 147(1), 156(0), 178(0), 209(1), 224(0), 292(21), 301(13), 304(2), 306(2), 307(2), 309(7), 313(3), 323(5), 325(4), 334(0), 339(12), 347(13), 363(16), 378(15), 383(18), 389(17), 392(22), 410(3), 420(6), 426(4), 434(34), 438(14), 442(16), 448(6), 459(6), 463(4), 475(38), 495(12), 500(40), 510(3), 520(16), 538(10), 553(66), 576(1), 579(0), 583(2), 585(1), 587(0), 587(0), 787(49), 790(85), 795(133), 796(41), 804(12), 804(28), 810(8), 810(14), 814(2), 815(9), 818(1), 818(13), 818(0), 819(4), 820(10), 870(2), 873(3), 878(1), 884(7), 885(1), 889(1), 989(9), 991(8), 992(4), 996(5), 997(4), 998(8), 1041(2), 1043(1), 1046(0), 1046(0), 1046(0), 1048(0), 1106(2), 1107(0), 1108(0), 1224(0), 1226(0), 1227(0), 1359(1), 1361(0), 1363(0), 1367(2), 1368(2), 1372(1), 1407(1), 1409(4), 1409(3), 1413(1), 1414(4), 1418(3), 1731(504), 1748(547), 1832(349), 1862(162), 1889(891), 1909(505), 1928(623), 1974(1024), 3172(0), 3172(0), 3173(1), 3176(0), 3177(0), 3181(0), 3183(0), 3187(0), 3188(1), 3190(0), 3190(0), 3192(1), 3195(0), 3201(0), 3201(0)	14(1), 26(0), 33(0), 47(0), 52(0), 56(0), 66(0), 68(0), 71(0), 78(1), 79(0), 83(1), 90(0), 92(0), 95(0), 99(0), 100(1), 106(2), 110(0), 115(1), 126(0), 133(0), 136(2), 145(1), 156(0), 176(0), 204(1), 223(0), 287(18), 293(15), 297(1), 298(3), 300(2), 301(10), 307(4), 318(2), 319(6), 330(1), 335(9), 343(14), 361(16), 376(16), 381(19), 387(21), 390(19), 409(2), 417(6), 421(3), 432(29), 435(13), 438(15), 445(7), 457(10), 461(3), 474(39), 495(17), 500(45), 510(3), 521(17), 537(9), 553(72), 570(1), 573(0), 577(2), 579(1), 580(0), 581(0), 770(9), 778(54), 782(79), 789(124), 792(35), 793(16), 795(29), 798(10), 806(44), 812(1), 813(4), 814(1), 815(3), 816(0), 817(1), 857(3), 859(1), 860(3), 863(5), 869(0), 873(1), 989(9), 990(8), 991(5), 995(5), 996(3), 997(9), 1040(2), 1043(1), 1045(0), 1045(0), 1046(0), 1047(0), 1106(0), 1106(1), 1108(0), 1223(0), 1226(0), 1226(0), 1358(1), 1360(0), 1363(0), 1366(2), 1368(3), 1371(1), 1406(1), 1409(3), 1409(4), 1412(2), 1414(4), 1418(3), 1742(544), 1760(481), 1839(329), 1861(194), 1893(855), 1914(481), 1932(609), 1976(995), 3173(1), 3173(0), 3174(1), 3179(0), 3179(0), 3183(0), 3185(0), 3189(0), 3190(1), 3193(0), 3193(0), 3195(1), 3197(0), 3204(0), 3205(1)

Table S34 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Cp}_3\text{Nb}_3(\text{CO})_8$ 8-4

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
12(0), 33(1), 36(0), 52(1), 59(0), 62(0), 63(1), 73(0), 78(2), 80(0), 85(1), 90(0), 96(1), 98(0), 103(1), 105(0), 108(1), 109(3), 113(1), 125(2), 128(1), 132(0), 136(3), 143(0), 150(1), 153(2), 167(0), 169(2), 311(19), 319(17), 324(2), 328(6), 337(0), 338(6), 340(6), 347(1), 360(4), 363(4), 368(13), 374(10), 411(15), 421(6), 424(36), 431(2), 440(8), 444(45), 445(31), 451(8), 457(4), 462(18), 463(17), 477(5), 484(29), 498(25), 530(65), 544(42), 553(55), 560(58), 563(13), 567(5), 569(4), 607(0), 611(0), 612(1), 613(0), 618(0), 622(1), 811(45), 813(43), 821(30), 827(114), 833(9), 837(0), 842(10), 842(6), 844(2), 845(2), 847(4), 848(2), 850(7), 855(43), 876(56), 898(2), 909(0), 910(3), 928(1), 932(9), 944(1), 985(2), 1025(9), 1026(5), 1030(11), 1032(5), 1033(4), 1077(9), 1077(1), 1083(1), 1085(2), 1086(1), 1086(1), 1140(2), 1142(3), 1147(1), 1264(0), 1277(0), 1280(0), 1400(1), 1413(1), 1422(4), 1423(0), 1425(2), 1427(2), 1458(4), 1468(1), 1473(4), 1474(4), 1474(4), 1479(4), 1932(134), 1961(114), 1988(37), 1998(887), 2019(894), 2030(1862), 2058(1693), 2092(418), 3055(1), 3273(0), 3280(0), 3283(0), 3283(0), 3286(0), 3291(0), 3292(1), 3295(1), 3295(1), 3298(0), 3300(1), 3305(0), 3312(0), 3313(0)	19(0), 31(0), 38(1), 49(1), 60(0), 61(1), 63(1), 73(0), 78(0), 80(2), 85(1), 88(0), 96(1), 97(0), 101(1), 103(0), 109(1), 111(2), 113(3), 124(1), 129(0), 133(0), 137(2), 144(0), 151(1), 153(2), 167(0), 173(4), 298(20), 312(21), 318(3), 323(7), 331(2), 333(4), 335(5), 343(1), 354(5), 358(3), 362(10), 374(10), 406(15), 414(3), 419(27), 422(10), 436(13), 439(12), 442(58), 448(12), 451(2), 459(22), 462(17), 474(9), 482(26), 496(30), 527(67), 543(20), 547(96), 559(4), 562(19), 563(47), 568(4), 601(0), 606(0), 607(0), 608(1), 612(0), 619(1), 800(40), 803(34), 811(39), 820(95), 826(10), 827(16), 832(6), 837(26), 838(10), 841(17), 843(1), 844(1), 845(1), 846(26), 872(57), 887(2), 895(0), 898(3), 915(3), 927(7), 932(12), 981(3), 1024(8), 1025(5), 1028(12), 1031(3), 1033(6), 1075(7), 1076(4), 1083(1), 1084(2), 1084(2), 1085(1), 1140(1), 1142(1), 1147(0), 1261(0), 1275(0), 1280(0), 1399(1), 1414(1), 1422(4), 1423(1), 1427(2), 1427(2), 1457(4), 1467(1), 1472(7), 1473(4), 1474(2), 1480(4), 1911(222), 1963(120), 1993(43), 1997(945), 2024(841), 2037(1639), 2067(1644), 2097(445), 3053(0), 3273(0), 3282(0), 3283(0), 3285(0), 3287(0), 3292(0), 3294(1), 3298(1), 3298(2), 3300(1), 3302(1), 3307(0), 3312(0), 3315(0)	34(0), 38(1), 42(0), 48(1), 52(0), 56(0), 63(1), 70(1), 73(0), 78(1), 81(0), 86(0), 90(0), 93(0), 98(1), 99(2), 101(0), 104(0), 111(0), 114(2), 124(1), 129(0), 136(2), 140(1), 141(0), 151(1), 162(1), 210(6), 280(7), 295(45), 305(1), 306(9), 313(2), 315(3), 324(6), 326(3), 336(7), 339(9), 347(3), 359(5), 372(13), 390(4), 406(11), 407(10), 413(6), 422(32), 427(31), 436(9), 440(14), 441(11), 446(11), 457(11), 469(10), 478(59), 490(23), 511(31), 520(16), 528(3), 530(6), 536(24), 539(130), 575(0), 580(1), 581(1), 582(0), 584(0), 589(2), 776(18), 779(47), 781(56), 792(46), 793(59), 795(3), 801(21), 809(17), 810(7), 812(1), 813(1), 813(40), 814(1), 817(3), 826(31), 852(1), 862(1), 862(2), 877(5), 884(2), 896(3), 947(2), 984(5), 987(7), 988(12), 989(2), 996(5), 1036(8), 1037(2), 1044(2), 1045(2), 1046(2), 1048(0), 1094(2), 1098(3), 1101(1), 1212(0), 1223(0), 1230(0), 1334(1), 1351(1), 1357(5), 1358(1), 1362(2), 1365(1), 1393(4), 1404(5), 1405(1), 1407(3), 1412(2), 1416(4), 1723(260), 1812(222), 1863(325), 1879(54), 1902(462), 1915(1375), 1937(1904), 1959(365), 2976(1), 3163(0), 3173(0), 3173(0), 3174(0), 3179(0), 3182(0), 3185(0), 3188(1), 3188(0), 3191(0), 3193(1), 3195(1), 3202(0), 3204(0)	34(1), 35(0), 43(0), 46(1), 48(0), 52(0), 62(1), 71(0), 74(0), 78(1), 80(0), 84(1), 88(0), 91(1), 97(1), 98(2), 100(0), 102(0), 109(0), 113(2), 122(1), 128(1), 136(2), 140(1), 141(0), 149(1), 162(1), 216(5), 272(6), 288(44), 298(1), 300(9), 308(3), 310(3), 318(8), 321(2), 330(7), 332(8), 342(3), 358(3), 365(16), 386(4), 400(4), 403(13), 409(5), 418(31), 425(35), 434(8), 437(7), 438(21), 444(10), 454(13), 467(8), 474(60), 485(26), 508(34), 516(15), 528(3), 529(5), 536(7), 541(155), 569(0), 575(1), 575(1), 575(1), 579(0), 584(2), 765(15), 770(42), 772(54), 783(3), 786(9), 789(105), 792(16), 799(20), 804(47), 808(10), 810(1), 810(0), 812(0), 813(0), 822(36), 841(1), 849(2), 851(1), 869(3), 873(11), 884(3), 949(2), 983(5), 987(8), 987(2), 989(11), 994(5), 1036(9), 1038(1), 1043(2), 1044(3), 1046(0), 1047(1), 1094(2), 1098(2), 1101(1), 1211(0), 1223(0), 1228(0), 1334(1), 1352(1), 1357(2), 1358(4), 1361(2), 1366(1), 1393(4), 1403(6), 1405(2), 1407(3), 1412(3), 1416(4), 1732(250), 1811(226), 1867(323), 1882(49), 1906(473), 1920(1324), 1940(1877), 1962(327), 2983(1), 3164(0), 3174(0), 3175(0), 3175(0), 3181(0), 3183(0), 3188(1), 3191(1), 3191(0), 3193(1), 3195(1), 3198(1), 3205(0), 3207(0)

Table S35 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Cp}_3\text{Nb}_3(\text{CO})_7$ 7-1

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
35(0), 45(0), 61(0), 68(0), 73(0), 77(0), 80(1), 81(0), 88(1), 90(0), 94(1), 102(0), 104(1), 107(0), 109(1), 119(3), 121(1), 126(2), 129(1), 140(1), 150(2), 155(1), 160(0), 174(0), 269(4), 312(1), 314(2), 322(6), 329(2), 330(2), 337(4), 343(4), 353(5), 357(25), 359(3), 387(46), 391(55), 416(15), 426(41), 441(42), 443(12), 451(23), 452(1), 461(5), 468(12), 475(14), 484(10), 496(22), 502(5), 522(27), 523(13), 539(33), 559(38), 564(18), 574(29), 596(21), 611(0), 614(3), 615(0), 616(0), 618(1), 620(5), 816(75), 819(89), 828(70), 832(48), 843(3), 844(21), 846(11), 847(24), 847(2), 848(3), 849(8), 850(0), 851(0), 852(4), 862(41), 909(1), 912(1), 913(2), 927(2), 933(2), 945(1), 1027(5), 1029(6), 1032(5), 1037(7), 1038(6), 1039(12), 1082(3), 1083(1), 1083(2), 1085(4), 1086(3), 1089(1), 1147(1), 1150(0), 1151(0), 1278(0), 1278(0), 1280(0), 1418(2), 1419(3), 1419(2), 1430(2), 1432(4), 1435(3), 1470(3), 1470(2), 1474(3), 1474(3), 1478(1), 1479(2), 1522(110), 1958(53), 1976(213), 2000(1265), 2019(1835), 2035(1196), 2068(317), 3279(0), 3281(0), 3283(0), 3283(0), 3286(0), 3288(0), 3292(0), 3296(1), 3297(0), 3298(0), 3298(1), 3302(0), 3309(0), 3314(0), 3318(0)	35(0), 44(0), 60(0), 66(0), 71(0), 75(0), 79(0), 81(0), 87(1), 89(0), 93(1), 101(1), 102(0), 106(0), 108(1), 118(4), 121(1), 127(2), 127(1), 138(1), 148(2), 153(1), 159(1), 171(1), 254(4), 301(2), 308(1), 316(7), 322(3), 324(2), 332(3), 337(4), 346(3), 353(23), 355(3), 383(47), 387(55), 410(14), 422(44), 438(42), 438(16), 448(18), 448(1), 458(6), 464(12), 472(18), 480(9), 494(23), 498(6), 520(31), 521(9), 537(37), 557(40), 563(23), 573(29), 592(20), 604(0), 607(4), 610(0), 610(0), 613(0), 614(7), 807(65), 810(49), 817(63), 819(96), 830(6), 832(9), 833(9), 837(54), 843(7), 845(4), 847(0), 847(9), 848(0), 848(0), 852(41), 897(1), 898(2), 898(2), 910(2), 923(3), 933(2), 1027(5), 1029(6), 1031(5), 1037(6), 1037(7), 1038(12), 1081(3), 1082(0), 1083(2), 1084(5), 1086(3), 1088(1), 1147(1), 1150(0), 1151(0), 1277(0), 1279(0), 1280(0), 1418(2), 1419(4), 1419(2), 1429(1), 1432(3), 1435(3), 1470(3), 1470(3), 1473(3), 1475(3), 1478(2), 1479(2), 1541(120), 1963(36), 1979(224), 2006(1268), 2025(1784), 2040(1142), 2071(279), 3280(0), 3282(0), 3284(0), 3284(0), 3287(0), 3289(0), 3294(1), 3298(0), 3298(2), 3299(0), 3299(1), 3303(0), 3310(0), 3316(0), 3320(0)	33(0), 43(0), 57(0), 65(0), 67(0), 71(0), 76(0), 77(1), 83(1), 86(0), 90(1), 97(0), 99(0), 102(0), 105(1), 112(2), 115(2), 119(2), 122(0), 134(1), 142(2), 146(1), 155(0), 165(1), 251(4), 294(2), 296(4), 304(3), 308(2), 310(3), 315(3), 322(4), 329(5), 335(13), 340(6), 368(28), 369(48), 396(13), 405(31), 420(11), 424(42), 430(1), 433(20), 443(6), 449(5), 454(23), 465(8), 473(12), 481(7), 492(14), 498(21), 508(21), 529(27), 534(12), 544(21), 560(21), 578(0), 581(2), 583(0), 583(0), 585(1), 588(3), 778(67), 781(62), 787(59), 793(71), 801(6), 803(15), 804(10), 806(37), 812(25), 813(5), 815(7), 816(0), 817(0), 818(0), 820(18), 862(1), 864(1), 864(1), 878(2), 884(1), 893(1), 986(5), 989(5), 992(5), 996(7), 997(5), 998(13), 1043(3), 1043(1), 1044(3), 1045(5), 1046(2), 1049(2), 1100(2), 1103(0), 1105(1), 1225(0), 1226(0), 1228(0), 1353(1), 1354(1), 1355(4), 1365(2), 1367(3), 1371(2), 1405(2), 1406(2), 1409(3), 1410(2), 1414(1), 1414(2), 1433(81), 1843(85), 1858(182), 1880(1013), 1898(1436), 1911(1040), 1940(292), 3171(0), 3173(0), 3175(0), 3175(0), 3178(0), 3180(0), 3184(0), 3188(0), 3188(0), 3189(0), 3189(0), 3193(0), 3200(0), 3205(0), 3208(0)	32(0), 42(0), 56(0), 63(0), 65(0), 68(0), 75(0), 77(0), 81(0), 84(0), 88(1), 96(0), 96(0), 100(0), 103(1), 111(3), 114(1), 119(2), 120(0), 132(0), 140(2), 144(1), 155(0), 163(1), 237(4), 288(2), 289(4), 294(3), 300(3), 303(2), 310(2), 315(5), 322(4), 331(13), 334(3), 364(32), 367(44), 390(11), 400(35), 415(8), 421(41), 427(3), 431(23), 440(8), 445(5), 451(26), 463(8), 470(13), 478(7), 491(11), 496(24), 506(23), 528(29), 534(16), 543(21), 557(19), 571(0), 575(2), 577(0), 578(0), 580(0), 582(3), 768(35), 773(54), 778(52), 782(107), 787(4), 790(8), 791(9), 798(64), 806(55), 810(2), 812(0), 814(0), 815(0), 815(4), 816(0), 850(3), 851(1), 851(1), 861(1), 875(2), 881(1), 986(5), 988(5), 991(5), 996(7), 997(6), 997(12), 1042(0), 1042(3), 1043(3), 1045(4), 1046(2), 1048(1), 1100(1), 1103(0), 1104(0), 1224(0), 1226(0), 1227(0), 1353(1), 1354(1), 1355(4), 1364(1), 1367(3), 1370(2), 1405(3), 1405(2), 1409(3), 1410(3), 1414(2), 1415(1), 1451(86), 1846(91), 1862(166), 1884(996), 1902(1419), 1915(977), 1943(264), 3172(0), 3174(0), 3176(0), 3176(0), 3179(0), 3181(0), 3186(0), 3190(0), 3190(1), 3191(0), 3191(0), 3195(0), 3202(0), 3207(0), 3211(0)

Table S36 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Cp}_3\text{Nb}_3(\text{CO})_7$ 7-2

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
34(0), 43(0), 52(0), 55(0), 58(0), 66(0), 74(0), 79(1), 80(0), 87(1), 92(0), 94(0), 98(3), 103(1), 108(0), 110(1), 112(0), 117(1), 124(1), 135(2), 145(0), 149(0), 156(0), 164(0), 302(2), 313(5), 315(0), 317(10), 322(2), 326(1), 336(11), 339(2), 346(5), 357(2), 370(26), 390(56), 398(4), 420(5), 423(85), 434(9), 445(77), 447(1), 457(4), 463(4), 471(5), 473(2), 481(8), 490(7), 502(23), 522(6), 531(18), 537(48), 558(9), 561(15), 577(22), 599(8), 611(0), 611(1), 612(1), 614(1), 615(0), 620(7), 784(53), 807(98), 818(37), 821(10), 823(106), 827(33), 835(27), 844(5), 845(0), 846(2), 849(1), 849(6), 850(0), 851(1), 856(30), 890(1), 895(0), 911(1), 919(0), 920(0), 936(0), 1025(11), 1030(6), 1033(5), 1035(9), 1036(7), 1038(7), 1077(1), 1082(1), 1083(3), 1084(1), 1086(2), 1087(1), 1148(0), 1150(3), 1151(1), 1277(0), 1279(0), 1280(0), 1418(4), 1420(1), 1421(4), 1425(29), 1430(3), 1435(2), 1436(31), 1469(3), 1470(2), 1474(3), 1480(2), 1480(2), 1481(3), 1978(316), 1995(134), 2020(252), 2040(1337), 2047(1610), 2097(1204), 3276(0), 3280(0), 3280(0), 3283(0), 3284(0), 3285(0), 3293(0), 3294(1), 3294(0), 3296(0), 3299(0), 3300(0), 3306(1), 3310(1), 3317(0)	34(0), 43(0), 54(0), 55(0), 58(0), 66(0), 74(0), 78(1), 79(0), 85(1), 91(0), 92(0), 97(3), 103(1), 107(0), 109(1), 112(0), 117(1), 124(1), 135(2), 143(0), 148(0), 154(0), 163(0), 293(3), 307(5), 310(1), 311(7), 316(3), 321(2), 330(11), 332(1), 340(4), 354(3), 363(24), 388(56), 392(5), 415(5), 419(87), 429(8), 441(73), 444(7), 453(2), 460(7), 467(6), 470(2), 479(11), 488(6), 499(26), 520(9), 528(22), 535(48), 557(2), 559(23), 578(23), 595(6), 605(0), 606(0), 607(0), 608(3), 611(1), 616(8), 770(38), 793(49), 807(33), 809(30), 814(116), 818(64), 819(43), 827(7), 840(33), 842(0), 844(2), 846(0), 847(0), 848(5), 848(1), 875(0), 881(1), 894(0), 895(1), 907(0), 920(0), 1025(12), 1030(6), 1032(6), 1035(9), 1036(7), 1038(7), 1077(1), 1082(1), 1082(3), 1083(1), 1086(2), 1086(1), 1148(0), 1150(2), 1151(0), 1276(0), 1279(0), 1280(0), 1418(3), 1421(1), 1421(2), 1427(10), 1430(2), 1433(2), 1446(59), 1469(3), 1470(2), 1473(4), 1479(2), 1480(3), 1481(3), 1984(321), 2001(129), 2026(245), 2045(1286), 2051(1557), 2101(1190), 3278(0), 3280(0), 3282(0), 3283(0), 3286(0), 3286(0), 3294(0), 3295(1), 3296(0), 3297(0), 3300(0), 3301(0), 3308(1), 3313(1), 3317(0)	31(0), 38(0), 47(0), 50(0), 53(0), 59(0), 69(0), 74(1), 76(0), 81(0), 86(0), 88(0), 93(1), 98(1), 102(0), 105(1), 105(1), 116(2), 120(0), 128(1), 137(0), 142(0), 146(0), 156(0), 285(1), 290(4), 295(1), 299(5), 302(3), 307(2), 314(4), 317(5), 327(5), 336(1), 356(23), 374(43), 377(4), 398(2), 406(69), 411(6), 422(34), 428(24), 436(1), 442(6), 449(11), 456(3), 458(7), 468(3), 476(12), 494(12), 504(43), 507(14), 528(8), 532(12), 548(15), 563(7), 578(0), 580(0), 580(0), 583(3), 584(1), 587(4), 744(33), 765(67), 778(58), 780(107), 781(13), 785(39), 792(33), 795(11), 806(22), 811(0), 813(0), 815(0), 816(0), 817(2), 818(1), 843(0), 846(1), 861(1), 868(0), 870(0), 879(1), 983(12), 988(3), 991(6), 994(8), 994(6), 998(8), 1038(2), 1042(2), 1042(2), 1044(1), 1047(1), 1048(1), 1101(1), 1103(3), 1104(1), 1223(0), 1227(0), 1227(0), 1346(43), 1353(1), 1355(2), 1356(4), 1365(1), 1366(2), 1369(3), 1404(3), 1406(2), 1409(3), 1414(1), 1415(4), 1415(1), 1862(249), 1877(97), 1901(258), 1917(1009), 1923(1390), 1970(1010), 3167(0), 3170(0), 3172(0), 3175(0), 3176(0), 3177(0), 3183(0), 3185(0), 3185(0), 3188(0), 3190(0), 3191(0), 3197(1), 3199(1), 3206(0)	28(0), 37(0), 45(0), 49(0), 52(0), 59(0), 67(0), 71(1), 77(0), 78(1), 84(0), 86(0), 91(1), 97(2), 99(0), 104(1), 104(0), 114(2), 118(0), 125(1), 134(0), 141(0), 145(0), 155(0), 275(2), 283(4), 289(1), 292(3), 294(5), 301(3), 307(3), 311(5), 321(4), 333(1), 346(20), 370(45), 372(4), 394(1), 402(72), 407(6), 417(36), 425(21), 432(1), 439(8), 447(15), 454(2), 456(10), 466(3), 474(13), 492(16), 503(38), 505(19), 528(6), 531(16), 548(16), 560(6), 572(0), 573(0), 575(0), 577(3), 578(2), 583(4), 730(20), 751(44), 768(4), 769(51), 771(71), 776(83), 779(80), 783(18), 793(28), 807(0), 811(0), 811(0), 812(0), 814(0), 815(1), 829(1), 834(1), 847(1), 848(0), 857(0), 864(0), 982(12), 987(3), 990(6), 994(7), 995(8), 998(9), 1038(2), 1041(1), 1042(3), 1044(1), 1046(1), 1048(1), 1101(1), 1104(1), 1104(2), 1223(0), 1226(0), 1226(0), 1354(4), 1354(5), 1356(2), 1359(24), 1365(2), 1368(1), 1369(22), 1403(4), 1406(2), 1408(3), 1414(2), 1415(5), 1415(1), 1867(247), 1881(97), 1906(249), 1921(973), 1926(1340), 1973(985), 3169(0), 3172(0), 3174(0), 3175(0), 3178(0), 3178(0), 3186(0), 3187(0), 3187(0), 3189(0), 3191(0), 3193(0), 3200(1), 3201(1), 3208(0)

Table S37 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Cp}_3\text{Nb}_3(\text{CO})_7$ 7-3

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
-52(2), -52(2), 57(1), 57(1), 59(1), 80(1), 80(1), 80(0), 84(0), 86(1), 86(1), 94(0), 108(0), 108(0), 113(0), 113(0), 120(0), 134(0), 134(0), 136(0), 159(0), 163(4), 163(4), 180(0), 180(0), 184(0), 217(3), 217(3), 302(0), 318(2), 318(2), 319(6), 327(3), 331(1), 331(1), 343(13), 343(13), 349(1), 413(45), 419(27), 419(27), 429(55), 429(55), 437(1), 450(24), 450(24), 455(7), 505(6), 505(6), 506(0), 514(1), 517(23), 517(23), 573(0), 579(11), 579(11), 610(1), 611(2), 611(2), 618(2), 618(2), 618(0), 828(184), 828(184), 829(6), 839(20), 839(20), 840(1), 846(2), 847(12), 847(12), 849(0), 849(2), 849(2), 852(9), 852(5), 852(5), 915(0), 915(0), 915(0), 934(0), 934(2), 934(2), 1032(9), 1032(9), 1032(0), 1038(0), 1038(0), 1038(17), 1080(1), 1081(0), 1081(0), 1086(2), 1086(2), 1086(2), 1154(0), 1154(0), 1154(0), 1278(0), 1278(0), 1278(0), 1425(6), 1425(7), 1425(7), 1430(0), 1431(6), 1431(6), 1472(1), 1472(1), 1472(0), 1481(8), 1481(1), 1481(1), 1834(335), 1957(28), 1957(28), 1990(2121), 2007(1441), 2007(1441), 2050(62), 3280(0), 3280(0), 3280(0), 3286(0), 3286(0), 3286(0), 3296(1), 3296(1), 3296(1), 3297(1), 3297(0), 3297(0), 3309(0), 3309(0), 3309(0)	-53(2), -53(2), 58(1), 58(1), 59(1), 79(1), 79(1), 80(0), 82(1), 85(1), 85(1), 93(0), 106(0), 106(0), 111(0), 111(0), 119(0), 132(0), 132(0), 136(0), 157(0), 161(4), 161(4), 177(0), 177(0), 182(0), 215(3), 215(3), 296(0), 312(2), 312(2), 314(6), 321(3), 325(1), 325(1), 340(13), 340(13), 346(1), 409(42), 416(23), 416(23), 425(54), 425(54), 433(2), 447(30), 447(30), 453(8), 502(5), 502(5), 505(0), 510(1), 515(27), 515(27), 573(0), 579(12), 579(12), 604(1), 606(3), 606(3), 614(2), 614(2), 614(0), 822(175), 822(175), 823(9), 828(30), 828(30), 829(1), 839(9), 840(18), 840(18), 846(1), 846(3), 846(3), 846(1), 847(0), 847(0), 904(0), 904(0), 905(0), 921(0), 922(2), 922(2), 1031(9), 1031(9), 1032(0), 1037(0), 1037(0), 1038(19), 1079(2), 1080(0), 1080(0), 1085(2), 1085(2), 1085(2), 1154(0), 1154(0), 1154(0), 1277(0), 1277(0), 1277(0), 1425(5), 1425(8), 1425(8), 1430(0), 1431(5), 1431(5), 1473(2), 1473(2), 1473(0), 1481(1), 1481(1), 1481(9), 1854(332), 1963(38), 1963(38), 1995(2084), 2014(1388), 2014(1388), 2054(43), 3281(0), 3281(0), 3281(0), 3286(0), 3286(0), 3286(0), 3297(1), 3297(1), 3297(1), 3299(3), 3299(0), 3299(0), 3310(0), 3310(0), 3311(0)	-19(0), -19(0), 55(1), 55(1), 55(1), 72(1), 73(0), 73(0), 80(0), 87(1), 87(1), 88(0), 102(0), 102(0), 109(0), 109(0), 112(0), 127(0), 128(0), 128(0), 150(0), 159(2), 159(2), 174(0), 181(0), 181(0), 219(2), 219(2), 289(0), 296(2), 296(2), 299(11), 303(0), 305(2), 305(2), 320(8), 320(8), 329(0), 398(27), 399(41), 399(41), 406(20), 406(20), 409(0), 434(28), 434(28), 436(4), 477(0), 482(4), 482(4), 491(0), 494(12), 494(12), 539(0), 549(7), 549(7), 578(1), 579(2), 579(2), 586(0), 586(2), 586(2), 787(161), 787(161), 788(8), 794(26), 794(26), 795(0), 807(8), 808(24), 808(24), 815(0), 816(2), 816(2), 816(1), 817(0), 817(0), 865(0), 865(0), 866(0), 883(0), 883(2), 883(2), 992(8), 992(8), 992(0), 997(0), 997(0), 997(17), 1040(2), 1041(0), 1041(0), 1046(1), 1046(1), 1046(2), 1108(0), 1108(0), 1108(0), 1226(0), 1226(0), 1226(0), 1359(4), 1360(7), 1360(7), 1366(0), 1367(4), 1367(4), 1409(2), 1409(2), 1409(0), 1416(1), 1416(1), 1416(7), 1695(211), 1843(22), 1843(22), 1871(1668), 1889(1160), 1889(1160), 1924(36), 3172(0), 3172(0), 3172(1), 3177(0), 3177(0), 3177(0), 3187(0), 3187(0), 3187(0), 3188(0), 3188(0), 3188(0), 3200(0), 3200(0), 3200(0)	-23(0), -23(0), 55(1), 55(1), 55(1), 72(1), 73(0), 73(0), 78(0), 85(1), 85(1), 87(0), 100(0), 100(0), 108(0), 108(0), 111(0), 126(0), 126(0), 127(0), 147(0), 157(2), 157(2), 171(0), 179(0), 179(0), 216(2), 216(2), 283(0), 290(2), 290(2), 293(11), 297(0), 298(2), 298(2), 316(8), 316(8), 326(0), 394(26), 397(43), 397(43), 403(16), 403(16), 406(1), 432(32), 432(32), 434(5), 475(0), 480(4), 480(4), 488(1), 492(13), 492(13), 540(0), 549(8), 549(8), 572(0), 574(2), 574(2), 581(0), 581(2), 581(2), 781(130), 781(130), 781(11), 783(44), 783(44), 785(1), 797(7), 797(40), 797(40), 813(0), 814(2), 814(2), 814(1), 814(0), 814(0), 854(0), 854(0), 855(0), 870(0), 871(2), 871(2), 991(8), 991(8), 992(0), 996(0), 996(0), 996(18), 1040(2), 1040(0), 1040(0), 1045(1), 1045(1), 1045(2), 1108(0), 1108(0), 1108(0), 1225(0), 1225(0), 1225(0), 1359(4), 1360(8), 1360(8), 1366(0), 1366(4), 1366(4), 1409(2), 1409(2), 1409(0), 1416(1), 1416(1), 1416(8), 1711(206), 1848(24), 1848(24), 1876(1626), 1893(1121), 1893(1121), 1927(28), 3172(1), 3172(0), 3172(0), 3178(0), 3178(0), 3178(0), 3189(0), 3189(0), 3189(0), 3190(1), 3190(0), 3190(0), 3202(0), 3202(0), 3202(0)

Table S38 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Cp}_3\text{Nb}_3(\text{CO})_6$ 6-1

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
27(0), 34(0), 41(0), 48(0), 53(0), 61(1), 72(1), 82(0), 85(0), 91(1), 93(0), 99(0), 103(0), 108(0), 122(1), 129(2), 135(0), 140(1), 147(0), 172(0), 182(1), 193(1), 208(0), 263(3), 308(15), 313(2), 319(2), 327(3), 328(3), 330(1), 340(14), 343(14), 359(2), 368(1), 372(3), 409(26), 411(3), 426(65), 431(13), 439(19), 444(2), 463(26), 465(14), 486(3), 497(23), 529(10), 535(24), 543(1), 554(11), 561(26), 573(69), 611(0), 613(0), 614(0), 615(4), 616(0), 618(0), 823(203), 824(133), 826(38), 834(11), 839(29), 842(31), 846(7), 847(13), 849(1), 849(3), 850(3), 850(2), 850(4), 852(2), 853(3), 918(1), 918(1), 920(2), 926(0), 928(3), 929(1), 1029(7), 1031(7), 1034(5), 1038(7), 1039(11), 1041(6), 1080(1), 1081(1), 1082(1), 1084(1), 1085(1), 1087(0), 1154(1), 1154(0), 1154(0), 1277(0), 1277(0), 1279(0), 1422(1), 1424(2), 1429(2), 1430(2), 1431(0), 1432(1), 1471(4), 1471(1), 1474(3), 1478(2), 1480(3), 1481(3), 1809(897), 1880(195), 1891(935), 1928(1195), 1961(602), 2082(863), 3276(0), 3278(0), 3279(0), 3280(0), 3281(0), 3284(0), 3291(0), 3291(1), 3293(0), 3293(1), 3296(1), 3298(1), 3303(0), 3304(0), 3305(1)	25(0), 31(0), 36(0), 46(1), 51(0), 60(1), 71(0), 80(0), 84(0), 88(2), 92(0), 97(0), 101(0), 107(0), 120(1), 128(2), 133(0), 139(1), 145(0), 170(0), 178(1), 192(0), 204(0), 261(3), 299(16), 305(2), 312(2), 319(4), 321(3), 322(1), 334(14), 338(15), 353(2), 364(1), 367(4), 405(27), 408(5), 423(53), 427(19), 434(23), 439(4), 460(8), 461(32), 482(3), 492(25), 526(9), 533(21), 540(2), 552(13), 562(37), 571(69), 605(0), 607(1), 607(0), 609(5), 609(1), 612(0), 808(108), 810(63), 813(29), 816(90), 823(78), 826(15), 827(30), 830(31), 837(33), 846(1), 846(2), 847(0), 848(2), 849(0), 849(0), 897(4), 898(1), 899(1), 902(0), 907(2), 915(3), 1028(7), 1031(7), 1033(6), 1037(8), 1038(5), 1038(12), 1078(1), 1080(1), 1081(1), 1083(0), 1083(1), 1085(0), 1153(0), 1153(0), 1154(0), 1276(0), 1277(0), 1279(0), 1422(1), 1423(2), 1429(2), 1430(1), 1430(1), 1432(0), 1471(4), 1472(1), 1474(4), 1478(2), 1479(3), 1482(3), 1824(876), 1894(146), 1905(951), 1938(1189), 1971(584), 2087(837), 3276(0), 3279(0), 3280(0), 3281(0), 3281(0), 3285(0), 3292(0), 3293(1), 3295(0), 3295(2), 3299(1), 3300(2), 3305(0), 3307(0), 3308(1)	15(0), 28(0), 37(0), 42(1), 46(0), 59(1), 70(0), 76(0), 82(0), 87(1), 89(0), 96(0), 98(0), 103(0), 115(1), 123(2), 131(0), 135(0), 142(0), 161(0), 172(1), 184(1), 208(1), 247(4), 283(8), 290(2), 296(4), 302(1), 303(4), 306(1), 318(11), 320(8), 336(3), 343(1), 346(0), 386(6), 394(10), 402(48), 416(10), 417(9), 429(12), 443(2), 448(21), 461(3), 471(20), 500(3), 506(2), 510(14), 521(10), 530(13), 541(49), 579(1), 580(1), 581(1), 581(1), 582(0), 585(0), 782(137), 783(89), 787(71), 794(19), 796(10), 799(50), 804(7), 805(20), 809(43), 816(1), 816(0), 817(0), 817(1), 819(1), 820(1), 864(0), 868(1), 872(2), 875(0), 880(2), 881(2), 990(7), 992(7), 993(4), 997(8), 998(6), 999(10), 1040(1), 1042(1), 1043(1), 1045(0), 1045(1), 1048(0), 1107(0), 1108(1), 1108(0), 1225(0), 1225(0), 1226(0), 1358(2), 1359(1), 1365(3), 1367(0), 1367(0), 1368(0), 1408(4), 1408(1), 1409(3), 1415(2), 1415(3), 1416(3), 1709(666), 1760(385), 1784(485), 1810(802), 1840(556), 1947(710), 3166(0), 3170(0), 3170(0), 3171(0), 3172(0), 3174(0), 3181(0), 3182(0), 3184(0), 3184(1), 3186(0), 3188(0), 3194(0), 3195(0), 3195(0)	20(0), 27(0), 35(0), 38(1), 46(0), 58(1), 69(0), 74(0), 80(0), 85(1), 88(0), 95(0), 96(0), 101(0), 113(0), 121(2), 128(0), 133(0), 139(0), 160(0), 169(1), 182(0), 203(1), 245(4), 274(9), 281(2), 289(4), 294(1), 296(4), 299(1), 312(10), 315(8), 333(3), 338(0), 342(0), 383(6), 391(12), 398(46), 411(6), 413(13), 426(13), 440(3), 446(20), 458(3), 467(22), 498(3), 504(1), 508(11), 521(10), 530(19), 540(50), 573(0), 573(2), 574(1), 575(0), 576(1), 580(0), 767(74), 768(49), 774(38), 779(14), 782(57), 785(49), 787(30), 790(71), 797(64), 813(1), 814(0), 814(0), 815(2), 816(0), 816(0), 844(1), 850(1), 853(2), 856(0), 859(3), 868(2), 989(7), 992(7), 992(5), 996(9), 997(5), 998(10), 1040(1), 1041(1), 1042(1), 1044(0), 1045(1), 1047(0), 1106(0), 1107(1), 1108(0), 1223(0), 1225(0), 1225(0), 1358(1), 1358(2), 1365(3), 1366(1), 1367(0), 1367(0), 1408(4), 1409(1), 1409(3), 1414(2), 1415(3), 1416(3), 1723(643), 1773(360), 1796(484), 1819(778), 1850(548), 1951(684), 3167(0), 3171(0), 3171(0), 3172(0), 3173(0), 3176(0), 3183(0), 3185(0), 3186(0), 3187(1), 3189(0), 3191(1), 3196(0), 3198(0), 3198(1)

Table S39 Harmonic vibrational frequencies(cm^{-1}) and IR intensities (KM/Mole) of $\text{Cp}_3\text{Nb}_3(\text{CO})_6$ 6-2

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
22(0), 31(0), 34(1), 43(1), 49(0), 57(0), 69(0), 75(1), 78(0), 84(0), 90(0), 98(1), 98(0), 107(3), 116(1), 117(0), 119(0), 138(3), 140(3), 147(1), 156(1), 166(1), 216(7), 284(17), 295(14), 300(6), 308(7), 321(27), 330(1), 333(1), 337(23), 338(3), 350(11), 374(32), 393(3), 402(29), 409(16), 430(8), 437(3), 445(30), 446(8), 459(19), 475(6), 487(10), 504(6), 513(40), 516(9), 541(9), 544(28), 555(1), 606(0), 608(0), 613(2), 615(0), 616(1), 620(0), 673(123), 808(77), 811(72), 814(151), 814(28), 829(11), 832(58), 833(28), 838(2), 841(13), 847(0), 849(0), 850(0), 850(1), 852(5), 854(3), 902(0), 910(1), 913(1), 917(3), 920(2), 925(1), 1028(10), 1032(7), 1033(10), 1034(11), 1037(13), 1040(5), 1079(0), 1080(0), 1082(3), 1083(2), 1084(0), 1085(1), 1149(0), 1153(2), 1153(1), 1277(0), 1278(0), 1279(0), 1337(163), 1417(2), 1420(6), 1425(3), 1428(1), 1428(1), 1431(0), 1471(2), 1472(2), 1473(2), 1477(4), 1480(2), 1484(2), 1905(815), 1922(332), 2003(837), 2022(1338), 2074(560), 3270(0), 3277(1), 3278(0), 3278(0), 3279(0), 3283(0), 3288(1), 3291(1), 3291(0), 3292(1), 3293(0), 3296(0), 3303(0), 3305(0), 3308(0)	20(0), 28(0), 29(0), 41(0), 47(0), 56(0), 69(0), 75(1), 77(0), 82(0), 89(0), 96(1), 98(0), 106(2), 115(1), 116(0), 118(0), 136(2), 138(4), 145(1), 154(1), 165(1), 215(7), 277(15), 287(13), 295(7), 302(6), 315(22), 324(2), 327(1), 332(13), 334(9), 347(14), 372(37), 390(3), 398(22), 405(24), 426(7), 432(2), 441(36), 443(4), 454(24), 472(5), 483(12), 505(1), 511(43), 514(4), 541(9), 544(33), 554(1), 598(0), 602(0), 605(3), 608(0), 610(1), 615(0), 670(131), 792(32), 799(27), 804(54), 805(132), 812(47), 818(80), 820(31), 823(15), 827(33), 844(0), 845(0), 847(0), 847(0), 848(3), 852(2), 883(3), 888(0), 897(1), 903(2), 905(2), 907(1), 1027(10), 1030(8), 1032(10), 1034(11), 1036(14), 1041(5), 1078(0), 1080(0), 1080(3), 1083(1), 1083(1), 1084(1), 1148(0), 1153(1), 1153(0), 1277(0), 1278(0), 1278(0), 1362(169), 1417(2), 1420(7), 1424(3), 1427(1), 1428(0), 1431(0), 1470(2), 1471(2), 1473(2), 1478(4), 1480(2), 1484(2), 1920(781), 1936(290), 2007(866), 2028(1266), 2081(543), 3270(0), 3276(0), 3279(0), 3280(0), 3281(0), 3284(0), 3289(1), 3292(1), 3293(1), 3294(0), 3295(0), 3297(0), 3305(0), 3306(1), 3311(0)	21(0), 39(0), 41(0), 47(0), 54(1), 57(0), 64(0), 72(0), 78(1), 82(0), 87(0), 95(0), 98(1), 103(1), 105(2), 110(1), 114(1), 129(3), 138(0), 147(3), 156(1), 164(1), 213(1), 267(11), 272(5), 286(17), 296(4), 302(17), 311(2), 313(3), 321(21), 325(6), 332(4), 354(15), 369(18), 382(3), 388(5), 417(4), 421(14), 427(20), 436(15), 442(18), 446(13), 457(1), 480(16), 484(19), 493(43), 511(24), 517(5), 521(6), 576(1), 577(0), 580(0), 584(2), 586(0), 592(0), 620(148), 763(66), 774(33), 779(84), 783(106), 786(13), 791(12), 793(7), 795(38), 798(38), 814(0), 817(5), 818(2), 818(1), 819(0), 821(5), 855(1), 856(0), 859(1), 868(0), 870(1), 879(1), 990(14), 991(8), 994(10), 995(10), 995(9), 999(3), 1040(1), 1042(2), 1044(0), 1045(1), 1047(0), 1048(0), 1103(1), 1104(4), 1106(2), 1224(0), 1227(0), 1228(0), 1335(117), 1355(1), 1357(2), 1360(0), 1362(2), 1364(6), 1364(0), 1406(1), 1407(1), 1411(2), 1412(3), 1412(2), 1418(2), 1786(659), 1799(306), 1889(1059), 1895(416), 1944(781), 3162(1), 3169(0), 3170(0), 3170(0), 3171(0), 3174(1), 3180(1), 3180(0), 3183(0), 3183(0), 3184(0), 3189(1), 3193(0), 3194(0), 3197(0)	21(0), 36(0), 39(0), 47(0), 52(1), 56(0), 63(0), 72(0), 78(1), 81(0), 86(1), 93(0), 97(1), 102(2), 103(1), 107(1), 113(1), 126(2), 134(0), 144(4), 153(1), 162(1), 211(0), 258(10), 263(5), 281(18), 290(6), 298(12), 305(2), 307(4), 316(20), 320(6), 328(4), 351(14), 366(18), 377(2), 386(5), 413(5), 418(11), 424(20), 432(12), 437(24), 440(15), 451(1), 477(16), 482(20), 493(41), 509(27), 518(5), 521(6), 569(1), 572(0), 574(0), 578(2), 580(0), 586(0), 613(159), 749(41), 757(22), 771(43), 773(41), 774(76), 778(6), 780(19), 783(101), 787(61), 812(1), 812(8), 815(1), 815(0), 816(0), 818(3), 833(0), 843(0), 844(0), 853(0), 858(0), 861(1), 989(15), 991(7), 993(10), 994(7), 994(13), 999(4), 1039(1), 1041(2), 1043(0), 1045(1), 1047(1), 1047(0), 1103(0), 1104(3), 1107(1), 1224(0), 1227(0), 1227(0), 1354(1), 1358(0), 1359(6), 1362(21), 1362(2), 1363(1), 1368(99), 1406(1), 1407(1), 1411(3), 1412(4), 1413(3), 1418(2), 1797(652), 1810(270), 1894(1007), 1901(438), 1948(759), 3162(1), 3170(0), 3170(0), 3171(0), 3173(0), 3176(0), 3182(0), 3182(0), 3185(0), 3185(0), 3186(0), 3190(1), 3196(0), 3196(0), 3199(0)