Electronic Supplementary Information for Dalton Transactions

Unsaturated Trinuclear Ruthenium Carbonyls: Large Structural Differences between Analogous Carbonyl Derivatives of the First, Second, and Third Row Transition Metals

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Supporting Information

Tables S1 to S17. Coordinates of $Ru_3(CO)_n$ (n = 12, 11, 10, 9)

Tables S18 to S34. Harmonic frequencies (cm^{-1}) and infrared intensities (km/mol) of $Ru_3(CO)_n$ (n = 12, 11, 10, 9)

Tables S1A to S8A. Complete lists of the total energies (E, in hartrees), relative energies (ΔE, in kcal/mol), number of imaginary vibrational frequencies (Nimag), and ν(CO) frequencies for the $Ru_3(CO)_n$ (n = 12, 11, 10, 9) structures by the MPW1PW91 and BP86 method using the SDD and LANL2DZ basis sets..

Complete Gaussian 03 reference (Reference 29)

Table S1 Coordinates of $Ru_3(CO)_{12}$ **(12-1)** D_3

	MPW1PW91/SDD			MPW1PW91/LANL2DZ			BP86/SDD			BP86/LANL2DZ		
	0.000000	1.646977	0.000000	0.000000	1.650773	0.000000	0.000000	1.671803	0.000000	0.000000	1.676905	0.000000
	1.426324	-0.823488	0.000000	1.429612	-0.825387	0.000000	1.447824	-0.835902	0.000000	1.452242	-0.838452	0.000000
Ru	-1.426324	-0.823488	0.000000	-1.429612	-0.825387	0.000000	-1.447824	-0.835902	0.000000	-1.452242	-0.838452	0.000000
Ru	-0.641550	1.524974	1.825583	-0.654448	1.522376	1.833593	-0.669878	1.541061	1.827239	-0.681904	1.538934	1.834988
Ru	0.641550	1.524974	-1.825583	0.654448	1.522376	-1.833593	0.669878	1.541061	-1.827239	0.681904	1.538934	-1.834988
C	1.389740	2.867114	0.456839	1.401972	2.878408	0.465767	1.378728	2.905995	0.481155	1.388397	2.918801	0.489650
C	-1.389740	2.867114	-0.456839	-1.401972	2.878408	-0.465767	-1.378728	2.905995	-0.481155	-1.388397	2.918801	-0.489650
C	0.999891	-1.318085	-1.825583	0.991192	-1.327956	-1.833593	0.999659	-1.350662	-1.827239	0.991804	-1.360013	-1.834988
C	1.641441	-0.206888	1.825583	1.645640	-0.194420	1.833593	1.669537	-0.190399	1.827239	1.673708	-0.178921	1.834988
C	3.177863	-0.230007	-0.456839	3.193760	-0.225061	-0.465767	3.206030	-0.258984	-0.481155	3.221954	-0.257013	-0.489650
C	1.788124	-2.637107	0.456839	1.791789	-2.653347	0.465767	1.827301	-2.647011	0.481155	1.833557	-2.661787	0.489650
C	-1.641441	-0.206888	-1.825583	-1.645640	-0.194420	-1.833593	-1.669537	-0.190399	-1.827239	-1.673708	-0.178921	-1.834988
C	-0.999891	-1.318085	1.825583	-0.991192	-1.327956	1.833593	-0.999659	-1.350662	1.827239	-0.991804	-1.360013	1.834988
C	-1.788124	-2.637107	-0.456839	-1.791789	-2.653347	-0.465767	-1.827301	-2.647011	-0.481155	-1.833557	-2.661787	-0.489650
C	-3.177863	-0.230007	0.456839	-3.193760	-0.225061	0.465767	-3.206030	-0.258984	0.481155	-3.221954	-0.257013	0.489650
C	-1.028833	1.594856	2.907161	-1.046957	1.591451	2.913055	-1.072863	1.620129	2.921936	-1.089002	1.617815	2.927865
C	1.028833	1.594856	-2.907161	1.046957	1.591451	-2.913055	1.072863	1.620129	-2.921936	1.089002	1.617815	-2.927865
O	2.195803	3.628146	0.763559	2.209842	3.632993	0.781105	2.179558	3.692198	0.808498	2.188498	3.701110	0.825848
O	-2.195803	3.628146	-0.763559	-2.209842	3.632993	-0.781105	-2.179558	3.692198	-0.808498	-2.188498	3.701110	-0.825848
O	0.866769	-1.688423	-2.907161	0.854758	-1.702417	-2.913055	0.866641	-1.739191	-2.921936	0.856568	-1.752011	-2.927865
O	1.895602	0.093568	2.907161	1.901715	0.110966	2.913055	1.939505	0.119062	2.921936	1.945570	0.134196	2.927865
O	4.239968	0.087549	-0.763559	4.251185	0.097283	-0.781105	4.287316	0.041454	-0.808498	4.299504	0.044740	-0.825848
O	2.044164	-3.715694	0.763559	2.041344	-3.730276	0.781105	2.107758	-3.733652	0.808498	2.111006	-3.745850	0.825848
O	-1.895602	0.093568	-2.907161	-1.901715	0.110966	-2.913055	-1.939505	0.119062	-2.921936	-1.945570	0.134196	-2.927865
O	-0.866769	-1.688423	2.907161	-0.854758	-1.702417	2.913055	-0.866641	-1.739191	2.921936	-0.856568	-1.752011	2.927865
O	-2.044164	-3.715694	-0.763559	-2.041344	-3.730276	-0.781105	-2.107758	-3.733652	-0.808498	-2.111006	-3.745850	-0.825848
O	-4.239968	0.087549	0.763559	-4.251185	0.097283	0.781105	-4.287316	0.041454	0.808498	-4.299504	0.044740	0.825848

O O				

Table S2 Coordinates of $Ru_3(CO)_{12}$ (**12-2**) C_{2v}

	MPW1PW91/SDD			MPW1PW91/LANL2DZ			BP86/SDD			BP86/LANL2DZ		
Ru	0.000000	-1.394434	-0.838898	0.000000	-1.406249	-0.837586	0.000000	-1.414913	-0.854055	0.000000	-1.427540	-0.853620
Ru	0.000000	1.394434	-0.838898	0.000000	1.406249	-0.837586	0.000000	1.414913	-0.854055	0.000000	1.427540	-0.853620
Ru	0.000000	0.000000	1.638186	0.000000	0.000000	1.634545	0.000000	0.000000	1.668342	0.000000	0.000000	1.665605
C	-1.502811	0.000000	-1.403258	-1.508533	0.000000	-1.412090	-1.504809	0.000000	-1.443193	-1.512350	0.000000	-1.449167
C	1.502811	0.000000	-1.403258	1.508533	0.000000	-1.412090	1.504809	0.000000	-1.443193	1.512350	0.000000	-1.449167
C	0.000000	1.455599	2.872257	0.000000	1.468338	2.879165	0.000000	1.453200	2.914999	0.000000	1.462888	2.923429
C	1.423721	2.495262	-0.149833	1.435644	2.508117	-0.136630	1.426811	2.520537	-0.157401	1.437879	2.533700	-0.146425
C	-1.423721	2.495262	-0.149833	-1.435644	2.508117	-0.136630	-1.426811	2.520537	-0.157401	-1.437879	2.533700	-0.146425
C	-1.933291	0.000000	1.479541	-1.944685	0.000000	1.466570	-1.942408	0.000000	1.500909	-1.953279	0.000000	1.486951
C	0.000000	-1.455599	2.872257	0.000000	-1.468338	2.879165	0.000000	-1.453200	2.914999	0.000000	-1.462888	2.923429
C	1.933291	0.000000	1.479541	1.944685	0.000000	1.466570	1.942408	0.000000	1.500909	1.953279	0.000000	1.486951
C	-1.423721	-2.495262	-0.149833	-1.435644	-2.508117	-0.136630	-1.426811	-2.520537	-0.157401	-1.437879	-2.533700	-0.146425
C	0.000000	2.148712	-2.592219	0.000000	2.175711	-2.601361	0.000000	2.197775	-2.600041	0.000000	2.223262	-2.608349
C	1.423721	-2.495262	-0.149833	1.435644	-2.508117	-0.136630	1.426811	-2.520537	-0.157401	1.437879	-2.533700	-0.146425
C	0.000000	-2.148712	-2.592219	0.000000	-2.175711	-2.601361	0.000000	-2.197775	-2.600041	0.000000	-2.223262	-2.608349
O	-2.587803	0.000000	-1.843314	-2.588574	0.000000	-1.859497	-2.597577	0.000000	-1.907611	-2.601502	0.000000	-1.917503
O	2.587803	0.000000	-1.843314	2.588574	0.000000	-1.859497	2.597577	0.000000	-1.907611	2.601502	0.000000	-1.917503
O	0.000000	2.317709	3.632820	0.000000	2.335337	3.633095	0.000000	2.319086	3.699613	0.000000	2.331468	3.704087
O	2.240001	3.211839	0.224696	2.249849	3.222955	0.244683	2.247199	3.262149	0.217091	2.256869	3.273826	0.233020
O	-2.240001	3.211839	0.224696	-2.249849	3.222955	0.244683	-2.247199	3.262149	0.217091	-2.256869	3.273826	0.233020
O	-3.081236	0.000000	1.461242	-3.092289	0.000000	1.443273	-3.108863	0.000000	1.486704	-3.119400	0.000000	1.467756
O	0.000000	-2.317709	3.632820	0.000000	-2.335337	3.633095	0.000000	-2.319086	3.699613	0.000000	-2.331468	3.704087
O	3.081236	0.000000	1.461242	3.092289	0.000000	1.443273	3.108863	0.000000	1.486704	3.119400	0.000000	1.467756
O	-2.240001	-3.211839	0.224696	-2.249849	-3.222955	0.244683	-2.247199	-3.262149	0.217091	-2.256869	-3.273826	0.233020
O	0.000000	2.633950	-3.633703	0.000000	2.668245	-3.638778	0.000000	2.715995	-3.646931	0.000000	2.749066	-3.650893
O	2.240001	-3.211839	0.224696	2.249849	-3.222955	0.244683	2.247199	-3.262149	0.217091	2.256869	-3.273826	0.233020
O	0.000000	-2.633950	-3.633703	0.000000	-2.668245	-3.638778	0.000000	-2.715995	-3.646931	0.000000	-2.749066	-3.650893

Table S3 Coordinates of $Ru_3(CO)_{12}$ (**12-3**) D_{3h}

	MPW1PW91/SDD			MPW1PW91/LANL2DZ			BP86/SDD			BP86/LANL2DZ		
Ru	0.000000	1.654828	0.000000	0.000000	1.658462	0.000000	0.000000	1.680913	0.000000	0.000000	1.685336	0.000000
Ru	-1.433123	-0.827414	0.000000	-1.436270	-0.829231	0.000000	-1.455714	-0.840457	0.000000	-1.459544	-0.842668	0.000000
Ru	1.433123	-0.827414	0.000000	1.436270	-0.829231	0.000000	1.455714	-0.840457	0.000000	1.459544	-0.842668	0.000000
C	0.000000	1.627724	1.936359	0.000000	1.624690	1.947977	0.000000	1.647671	1.947182	0.000000	1.644280	1.958643
C	0.000000	1.627724	-1.936359	0.000000	1.624690	-1.947977	0.000000	1.647671	-1.947182	0.000000	1.644280	-1.958643
C	-1.490565	2.837585	0.000000	-1.506146	2.845995	0.000000	-1.489476	2.876985	0.000000	-1.503606	2.885929	0.000000
C	1.490565	2.837585	0.000000	1.506146	2.845995	0.000000	1.489476	2.876985	0.000000	1.503606	2.885929	0.000000
C	-1.409651	-0.813862	-1.936359	-1.407023	-0.812345	-1.947977	-1.426925	-0.823836	-1.947182	-1.423988	-0.822140	-1.958643
C	-1.409651	-0.813862	1.936359	-1.407023	-0.812345	1.947977	-1.426925	-0.823836	1.947182	-1.423988	-0.822140	1.958643
C	-3.202703	-0.127925	0.000000	-3.217777	-0.118637	0.000000	-3.236280	-0.148568	0.000000	-3.251090	-0.140803	0.000000
C	-1.712138	-2.709659	0.000000	-1.711631	-2.727358	0.000000	-1.746804	-2.728417	0.000000	-1.747485	-2.745125	0.000000
C	1.409651	-0.813862	-1.936359	1.407023	-0.812345	-1.947977	1.426925	-0.823836	-1.947182	1.423988	-0.822140	-1.958643
C	1.409651	-0.813862	1.936359	1.407023	-0.812345	1.947977	1.426925	-0.823836	1.947182	1.423988	-0.822140	1.958643
C	1.712138	-2.709659	0.000000	1.711631	-2.727358	0.000000	1.746804	-2.728417	0.000000	1.747485	-2.745125	0.000000
C	3.202703	-0.127925	0.000000	3.217777	-0.118637	0.000000	3.236280	-0.148568	0.000000	3.251090	-0.140803	0.000000
O	0.000000	1.777181	3.076252	0.000000	1.774618	3.087578	0.000000	1.807182	3.104233	0.000000	1.804878	3.115303
O	0.000000	1.777181	-3.076252	0.000000	1.774618	-3.087578	0.000000	1.807182	-3.104233	0.000000	1.804878	-3.115303
O	-2.370791	3.578453	0.000000	-2.391108	3.580146	0.000000	-2.372608	3.643281	0.000000	-2.390356	3.647031	0.000000
O	2.370791	3.578453	0.000000	2.391108	3.580146	0.000000	2.372608	3.643281	0.000000	2.390356	3.647031	0.000000
O	-1.539083	-0.888590	-3.076252	-1.536864	-0.887309	-3.087578	-1.565065	-0.903591	-3.104233	-1.563070	-0.902439	-3.115303
O	-1.539083	-0.888590	3.076252	-1.536864	-0.887309	3.087578	-1.565065	-0.903591	3.104233	-1.563070	-0.902439	3.115303
O	-4.284426	0.263939	0.000000	-4.296052	0.280687	0.000000	-4.341478	0.233098	0.000000	-4.353600	0.246594	0.000000
O	-1.913635	-3.842391	0.000000	-1.904943	-3.860834	0.000000	-1.968870	-3.876379	0.000000	-1.963243	-3.893625	0.000000
O	1.539083	-0.888590	-3.076252	1.536864	-0.887309	-3.087578	1.565065	-0.903591	-3.104233	1.563070	-0.902439	-3.115303
O	1.539083	-0.888590	3.076252	1.536864	-0.887309	3.087578	1.565065	-0.903591	3.104233	1.563070	-0.902439	3.115303
O	1.913635	-3.842391	0.000000	1.904943	-3.860834	0.000000	1.968870	-3.876379	0.000000	1.963243	-3.893625	0.000000
O	4.284426	0.263939	0.000000	4.296052	0.280687	0.000000	4.341478	0.233098	0.000000	4.353600	0.246594	0.000000

Table S4 Coordinates of $Ru_3(CO)_{12}$ (**12-4**) D_{3h}

	MPW1PW91/SDD			MPW1PW91/LANL2DZ			BP86/SDD			BP86/LANL2DZ		
Ru	0.000000	1.665481	0.000000	0.000000	1.682852	0.000000	0.000000	1.692789	0.000000	0.000000	1.710301	0.000000
Ru	-1.442349	-0.832741	0.000000	-1.457392	-0.841426	0.000000	-1.465998	-0.846395	0.000000	-1.481164	-0.855151	0.000000
Ru	1.442349	-0.832741	0.000000	1.457392	-0.841426	0.000000	1.465998	-0.846395	0.000000	1.481164	-0.855151	0.000000
C	2.084859	1.203694	0.000000	2.099770	1.212303	0.000000	2.091944	1.207784	0.000000	2.107205	1.216595	0.000000
C	0.000000	-2.407388	0.000000	0.000000	-2.424605	0.000000	0.000000	-2.415569	0.000000	0.000000	-2.433190	0.000000
C	-2.084859	1.203694	0.000000	-2.099770	1.212303	0.000000	-2.091944	1.207784	0.000000	-2.107205	1.216595	0.000000
C	0.000000	1.772623	1.939810	0.000000	1.772763	1.951450	0.000000	1.804472	1.947110	0.000000	1.802841	1.958101
C	0.000000	1.772623	-1.939810	0.000000	1.772763	-1.951450	0.000000	1.804472	-1.947110	0.000000	1.802841	-1.958101
C	-1.535137	-0.886312	-1.939810	-1.535258	-0.886381	-1.951450	-1.562719	-0.902236	-1.947110	-1.561306	-0.901421	-1.958101
C	-1.535137	-0.886312	1.939810	-1.535258	-0.886381	1.951450	-1.562719	-0.902236	1.947110	-1.561306	-0.901421	1.958101
C	1.535137	-0.886312	-1.939810	1.535258	-0.886381	-1.951450	1.562719	-0.902236	-1.947110	1.561306	-0.901421	-1.958101
C	1.535137	-0.886312	1.939810	1.535258	-0.886381	1.951450	1.562719	-0.902236	1.947110	1.561306	-0.901421	1.958101
C	0.000000	3.549322	0.000000	0.000000	3.579225	0.000000	0.000000	3.583547	0.000000	0.000000	3.611161	0.000000
C	-3.073803	-1.774661	0.000000	-3.099699	-1.789612	0.000000	-3.103443	-1.791773	0.000000	-3.127357	-1.805581	0.000000
C	3.073803	-1.774661	0.000000	3.099699	-1.789612	0.000000	3.103443	-1.791773	0.000000	3.127357	-1.805581	0.000000
O	3.096144	1.787560	0.000000	3.109611	1.795335	0.000000	3.118818	1.800650	0.000000	3.132565	1.808587	0.000000
O	0.000000	-3.575120	0.000000	0.000000	-3.590670	0.000000	0.000000	-3.601301	0.000000	0.000000	-3.617175	0.000000
O	-3.096144	1.787560	0.000000	-3.109611	1.795335	0.000000	-3.118818	1.800650	0.000000	-3.132565	1.808587	0.000000
O	0.000000	1.923630	3.076296	0.000000	1.905445	3.089865	0.000000	1.970844	3.100445	0.000000	1.949568	3.113693
O	0.000000	1.923630	-3.076296	0.000000	1.905445	-3.089865	0.000000	1.970844	-3.100445	0.000000	1.949568	-3.113693
O	-1.665912	-0.961815	-3.076296	-1.650163	-0.952722	-3.089865	-1.706801	-0.985422	-3.100445	-1.688376	-0.974784	-3.113693
O	-1.665912	-0.961815	3.076296	-1.650163	-0.952722	3.089865	-1.706801	-0.985422	3.100445	-1.688376	-0.974784	3.113693
O	1.665912	-0.961815	-3.076296	1.650163	-0.952722	-3.089865	1.706801	-0.985422	-3.100445	1.688376	-0.974784	-3.113693
O	1.665912	-0.961815	3.076296	1.650163	-0.952722	3.089865	1.706801	-0.985422	3.100445	1.688376	-0.974784	3.113693
O	0.000000	4.701072	0.000000	0.000000	4.730538	0.000000	0.000000	4.754308	0.000000	0.000000	4.781592	0.000000
O	-4.071248	-2.350536	0.000000	-4.096766	-2.365269	0.000000	-4.117352	-2.377154	0.000000	-4.140980	-2.390796	0.000000
O	4.071248	-2.350536	0.000000	4.096766	-2.365269	0.000000	4.117352	-2.377154	0.000000	4.140980	-2.390796	0.000000

Table S5 Coordinates of $Ru_3(CO)_{11}$ (**11-1**)

	MPW1PW91/SDD			MPW1PW91/LANL2DZ			BP86/SDD			BP86/LANL2DZ		
Ru	0.862712	1.181211	-0.225674	0.844889	1.191555	-0.239949	0.895498	1.203339	-0.227125	0.873575	1.216435	-0.243209
Ru	-1.629656	-0.078751	0.111657	-1.630559	-0.095927	0.116780	-1.642257	-0.057079	0.109858	-1.645753	-0.079953	0.114461
Ru	0.797074	-1.552827	0.288581	0.831757	-1.548791	0.306272	0.781251	-1.570645	0.284420	0.823036	-1.566777	0.306076
C	0.499440	1.612768	1.636954	0.493812	1.644548	1.633277	0.590018	1.642390	1.655808	0.586133	1.682341	1.649314
C	0.974132	0.496849	-2.038142	0.942450	0.478249	-2.054761	0.955240	0.481743	-2.036071	0.917528	0.456056	-2.048339
C	2.740424	1.569116	-0.135059	2.735923	1.619812	-0.180875	2.783836	1.575166	-0.182657	2.769625	1.639648	-0.239009
C	0.274774	2.895025	-0.778062	0.201455	2.893505	-0.808201	0.328565	2.929036	-0.785942	0.241579	2.924619	-0.822618
C	-1.891704	0.377335	-1.768870	-1.918364	0.335616	-1.783476	-1.962802	0.463792	-1.755676	-1.995320	0.399576	-1.774206
C	-0.995878	-0.850667	1.782554	-0.966554	-0.836121	1.804094	-0.927147	-0.894290	1.754274	-0.894118	-0.864329	1.781551
C	-3.115565	-1.268968	0.092500	-3.108250	-1.319939	0.129988	-3.184394	-1.187114	0.135463	-3.176858	-1.244744	0.186133
C	-2.547506	1.412849	0.851710	-2.571143	1.404138	0.849829	-2.491385	1.428211	0.948584	-2.517850	1.419889	0.931474
C	-0.284531	-2.105461	-1.248199	-0.270677	-2.141487	-1.214254	-0.417875	-2.123398	-1.181628	-0.390578	-2.170341	-1.142046
C	1.821122	-0.998297	1.814236	1.871283	-0.944203	1.817921	1.918775	-1.057712	1.752886	1.975382	-0.990542	1.754202
C	2.375644	-2.142240	-0.537562	2.417915	-2.131428	-0.539987	2.283319	-2.277115	-0.624670	2.334016	-2.267777	-0.616489
O	0.334206	1.946782	2.722872	0.332889	1.987295	2.716542	0.459887	1.979122	2.764490	0.460510	2.032086	2.753859
O	1.107030	0.136213	-3.119569	1.066785	0.103332	-3.131992	1.060706	0.104638	-3.134662	1.016500	0.058903	-3.140192
O	3.854737	1.836961	-0.060697	3.845544	1.906973	-0.122962	3.919397	1.843077	-0.140877	3.897601	1.937340	-0.221688
O	-0.080120	3.927013	-1.140071	-0.191711	3.907674	-1.179213	-0.012683	3.982328	-1.160241	-0.142936	3.957365	-1.210363
O	-2.157722	0.666229	-2.850800	-2.201187	0.610484	-2.864142	-2.276914	0.797826	-2.831191	-2.328754	0.709623	-2.850399
O	-0.992248	-1.268982	2.872795	-0.954272	-1.227923	2.903031	-0.947872	-1.333127	2.858294	-0.898531	-1.263718	2.899098
O	-4.037787	-1.956135	0.061990	-4.015959	-2.025684	0.116887	-4.158457	-1.833871	0.135039	-4.136897	-1.910625	0.213909
O	-3.137561	2.277651	1.330620	-3.164980	2.267856	1.324645	-3.060604	2.300157	1.482417	-3.093238	2.295092	1.452140
O	-0.774372	-2.621390	-2.157855	-0.764109	-2.678033	-2.109489	-0.945499	-2.693774	-2.062685	-0.916640	-2.763733	-2.007725
O	2.493653	-0.750808	2.714985	2.549429	-0.669247	2.705812	2.664133	-0.850842	2.630660	2.727249	-0.749029	2.616791
O	3.336704	-2.465249	-1.088415	3.373206	-2.442352	-1.106354	3.201088	-2.696949	-1.220862	3.248265	-2.674978	-1.225709

Table S6 Coordinates of $Ru_3(CO)_{11}$ (**11-2**)

	MPW1PW91/SDD			MPW1PW91/LANL2DZ			BP86/SDD			BP86/LANL2DZ		
Ru	1.232654	-0.841004	0.000000	1.242470	-0.831951	0.000000	1.258160	-0.867431	0.000000	1.273239	-0.849250	0.000000
Ru	-0.150240	1.669376	0.000000	-0.160984	1.672032	0.000000	-0.130489	1.687350	0.000000	-0.151153	1.691375	0.000000
Ru	-1.548437	-0.833957	0.000000	-1.554260	-0.854483	0.000000	-1.560519	-0.837847	0.000000	-1.564880	-0.865507	0.000000
C	1.203521	-0.802385	1.940937	1.215406	-0.786825	1.953083	1.203282	-0.848228	1.950314	1.223496	-0.817861	1.961951
C	1.203521	-0.802385	-1.940937	1.215406	-0.786825	-1.953083	1.203282	-0.848228	-1.950314	1.223496	-0.817861	-1.961951
C	1.656759	-2.705948	0.000000	1.698669	-2.708575	0.000000	1.715925	-2.730372	0.000000	1.754109	-2.722702	0.000000
C	2.973497	-0.092156	0.000000	2.975371	-0.036644	0.000000	3.001056	-0.105823	0.000000	3.011332	-0.050833	0.000000
C	-0.174203	1.635693	-1.933105	-0.177566	1.638883	-1.945444	-0.125407	1.649297	-1.944570	-0.147110	1.651101	-1.956142
C	-0.174203	1.635693	1.933105	-0.177566	1.638883	1.945444	-0.125407	1.649297	1.944570	-0.147110	1.651101	1.956142
C	-1.762756	2.665776	0.000000	-1.829402	2.601049	0.000000	-1.769416	2.658565	0.000000	-1.837427	2.604929	0.000000
C	1.250331	2.977826	0.000000	1.211599	3.034281	0.000000	1.236690	3.041128	0.000000	1.188771	3.092455	0.000000
C	-1.667601	-0.816071	-1.925945	-1.654373	-0.831617	-1.938357	-1.727469	-0.786896	-1.927858	-1.700210	-0.820098	-1.941676
C	-1.667601	-0.816071	1.925945	-1.654373	-0.831617	1.938357	-1.727469	-0.786896	1.927858	-1.700210	-0.820098	1.941676
C	-1.824011	-2.671995	0.000000	-1.801700	-2.709175	0.000000	-1.886081	-2.678152	0.000000	-1.868147	-2.720925	0.000000
O	1.312393	-0.878496	3.081086	1.330598	-0.860668	3.092502	1.293069	-0.951303	3.108510	1.326425	-0.913309	3.119474
O	1.312393	-0.878496	-3.081086	1.330598	-0.860668	-3.092502	1.293069	-0.951303	-3.108510	1.326425	-0.913309	-3.119474
O	1.953621	-3.815655	0.000000	2.014281	-3.812329	0.000000	2.053668	-3.848324	0.000000	2.105131	-3.835807	0.000000
O	4.028553	0.365263	0.000000	4.016028	0.451482	0.000000	4.072077	0.362139	0.000000	4.070981	0.441099	0.000000
O	-0.198521	1.771652	-3.075909	-0.199515	1.776352	-3.087669	-0.127648	1.793948	-3.104818	-0.156148	1.798114	-3.115694
O	-0.198521	1.771652	3.075909	-0.199515	1.776352	3.087669	-0.127648	1.793948	3.104818	-0.156148	1.798114	3.115694
O	-2.731511	3.290615	0.000000	-2.828615	3.174999	0.000000	-2.763432	3.277946	0.000000	-2.857255	3.179812	0.000000
O	2.040270	3.815287	0.000000	1.970451	3.899130	0.000000	2.003053	3.925122	0.000000	1.924875	4.001030	0.000000
O	-1.898993	-0.871314	-3.051701	-1.866456	-0.884376	-3.067514	-2.022781	-0.808936	-3.059886	-1.961346	-0.854238	-3.081065
O	-1.898993	-0.871314	3.051701	-1.866456	-0.884376	3.067514	-2.022781	-0.808936	3.059886	-1.961346	-0.854238	3.081065
O	-1.920501	-3.824461	0.000000	-1.867248	-3.863054	0.000000	-2.019228	-3.845964	0.000000	-1.976971	-3.890571	0.000000

Table S7 Coordinates of $Ru_3(CO)_{11}$ (**11-3**)

	MPW1PW91/SDD			MPW1PW91/LANL2DZ			BP86/SDD			BP86/LANL2DZ		
Ru	0.000000	1.655460	-0.898303	0.000000	1.670883	-0.908854	0.000000	1.659519	-0.901014	0.000000	1.676970	-0.913238
Ru	0.000000	-1.655460	-0.898303	0.000000	-1.670883	-0.908854	0.000000	-1.659519	-0.901014	0.000000	-1.676970	-0.913238
Ru	0.000000	0.000000	1.424764	0.000000	0.000000	1.437316	0.000000	0.000000	1.461637	0.000000	0.000000	1.471186
C	-1.934146	1.621379	-1.079151	-1.946433	1.630756	-1.067653	-1.934383	1.602666	-1.119359	-1.947325	1.614539	-1.103584
C	1.934146	1.621379	-1.079151	1.946433	1.630756	-1.067653	1.934383	1.602666	-1.119359	1.947325	1.614539	-1.103584
C	0.000000	2.088916	1.066371	0.000000	2.097458	1.076540	0.000000	2.102525	1.075258	0.000000	2.112858	1.082151
C	0.000000	3.349970	-1.709152	0.000000	3.362771	-1.754282	0.000000	3.363189	-1.713223	0.000000	3.377667	-1.755874
C	1.934146	-1.621379	-1.079151	1.946433	-1.630756	-1.067653	1.934383	-1.602666	-1.119359	1.947325	-1.614539	-1.103584
C	-1.934146	-1.621379	-1.079151	-1.946433	-1.630756	-1.067653	-1.934383	-1.602666	-1.119359	-1.947325	-1.614539	-1.103584
C	0.000000	-2.088916	1.066371	0.000000	-2.097458	1.076540	0.000000	-2.102525	1.075258	0.000000	-2.112858	1.082151
C	0.000000	-3.349970	-1.709152	0.000000	-3.362771	-1.754282	0.000000	-3.363189	-1.713223	0.000000	-3.377667	-1.755874
C	1.938277	0.000000	1.467073	1.950196	0.000000	1.471403	1.947104	0.000000	1.507789	1.958067	0.000000	1.508629
C	-1.938277	0.000000	1.467073	-1.950196	0.000000	1.471403	-1.947104	0.000000	1.507789	-1.958067	0.000000	1.508629
C	0.000000	0.000000	3.318335	0.000000	0.000000	3.346734	0.000000	0.000000	3.359705	0.000000	0.000000	3.382157
O	-3.064919	1.638847	-1.274399	-3.080282	1.637836	-1.242214	-3.077019	1.615927	-1.356146	-3.094498	1.618269	-1.314582
O	3.064919	1.638847	-1.274399	3.080282	1.637836	-1.242214	3.077019	1.615927	-1.356146	3.094498	1.618269	-1.314582
O	0.000000	3.103516	1.659100	0.000000	3.114848	1.660576	0.000000	3.129023	1.681821	0.000000	3.140711	1.682544
O	0.000000	4.417676	-2.144721	0.000000	4.424549	-2.203038	0.000000	4.444757	-2.164237	0.000000	4.453990	-2.218485
O	3.064919	-1.638847	-1.274399	3.080282	-1.637836	-1.242214	3.077019	-1.615927	-1.356146	3.094498	-1.618269	-1.314582
O	-3.064919	-1.638847	-1.274399	-3.080282	-1.637836	-1.242214	-3.077019	-1.615927	-1.356146	-3.094498	-1.618269	-1.314582
O	0.000000	-3.103516	1.659100	0.000000	-3.114848	1.660576	0.000000	-3.129023	1.681821	0.000000	-3.140711	1.682544
O	0.000000	-4.417676	-2.144721	0.000000	-4.424549	-2.203038	0.000000	-4.444757	-2.164237	0.000000	-4.453990	-2.218485
O	3.080443	0.000000	1.578883	3.092535	0.000000	1.576055	3.106660	0.000000	1.632939	3.117840	0.000000	1.627434
O	-3.080443	0.000000	1.578883	-3.092535	0.000000	1.576055	-3.106660	0.000000	1.632939	-3.117840	0.000000	1.627434
O	0.000000	0.000000	4.468470	0.000000	0.000000	4.496239	0.000000	0.000000	4.529252	0.000000	0.000000	4.551215

Table S8 Coordinates of $Ru_3(CO)_{11}$ (**11-4**)

	MPW1PW91/SDD			MPW1PW91/LANL2DZ			BP86/SDD			BP86/LANL2DZ		
Ru	1.628880	0.000000	-0.027834	0.029027	1.636040	0.000000	0.025011	1.657729	0.000000	1.668464	0.000000	-0.022030
Ru	-0.862841	-1.320431	0.037405	-0.040001	-0.867300	1.322493	-0.037128	-0.875631	1.341428	-0.880403	-1.345131	0.037697
Ru	-0.862841	1.320431	0.037405	-0.040001	-0.867300	-1.322493	-0.037128	-0.875631	-1.341428	-0.880403	1.345131	0.037697
C	2.733185	0.000000	1.592776	-1.616101	2.736857	0.000000	-1.588322	2.780570	0.000000	2.781783	0.000000	1.618181
C	2.602520	1.456779	-0.799544	0.796503	2.620803	-1.471315	0.799854	2.638095	-1.460006	2.663645	1.472753	-0.787637
C	2.602520	-1.456779	-0.799544	0.796503	2.620803	1.471315	0.799854	2.638095	1.460006	2.663644	-1.472753	-0.787637
C	-0.731422	-2.649349	1.398551	-1.415378	-0.770789	2.657933	-1.395125	-0.744024	2.679676	-0.821504	-2.679751	1.418428
C	-0.497164	-2.685856	-1.242898	1.232817	-0.465545	2.702399	1.246534	-0.517295	2.713458	-0.464389	-2.740127	-1.221055
C	-2.763496	-1.405672	-0.160869	0.203768	-2.780486	1.395711	0.154379	-2.784676	1.415753	-2.796525	-1.401609	-0.229064
C	-0.731422	2.649349	1.398551	-1.415378	-0.770789	-2.657933	-1.395125	-0.744024	-2.679676	-0.821504	2.679751	1.418428
C	-2.763496	1.405672	-0.160869	0.203768	-2.780486	-1.395711	0.154379	-2.784676	-1.415753	-2.796525	1.401609	-0.229064
C	-0.497163	2.685856	-1.242898	1.232817	-0.465545	-2.702399	1.246534	-0.517295	-2.713458	-0.464389	2.740127	-1.221055
C	0.112757	0.000000	1.488546	-1.505901	0.098841	0.000000	-1.489136	0.117494	0.000000	0.102495	0.000000	1.503517
C	0.307969	0.000000	-1.546859	1.565437	0.329487	0.000000	1.549482	0.307389	0.000000	0.341642	0.000000	-1.570172
O	3.422099	0.000000	2.508583	-2.531867	3.424856	0.000000	-2.508393	3.494996	0.000000	3.493495	0.000000	2.539557
O	3.172043	2.332387	-1.279158	1.272344	3.191891	-2.347276	1.284835	3.224014	-2.346709	3.256224	2.357097	-1.267475
O	3.172042	-2.332387	-1.279158	1.272344	3.191891	2.347276	1.284835	3.224014	2.346709	3.256224	-2.357097	-1.267475
O	-0.674216	-3.422679	2.244508	-2.267348	-0.737674	3.425477	-2.252067	-0.693786	3.470428	-0.822740	-3.458730	2.287187
O	-0.298023	-3.497440	-2.030424	2.009238	-0.244243	3.518453	2.046547	-0.329065	3.542981	-0.241058	-3.580618	-1.999972
O	-3.892483	-1.593891	-0.270793	0.342261	-3.904572	1.591771	0.259786	-3.931630	1.615649	-3.936433	-1.609531	-0.381345
O	-0.674216	3.422679	2.244508	-2.267348	-0.737674	-3.425477	-2.252067	-0.693786	-3.470428	-0.822740	3.458730	2.287187
O	-3.892483	1.593892	-0.270793	0.342261	-3.904572	-1.591771	0.259786	-3.931630	-1.615649	-3.936433	1.609531	-0.381345
O	-0.298023	3.497440	-2.030424	2.009238	-0.244243	-3.518453	2.046547	-0.329065	-3.542981	-0.241058	3.580618	-1.999972
O	0.084207	0.000000	2.676463	-2.690263	0.077147	0.000000	-2.694286	0.069388	0.000000	0.058901	0.000000	2.705288
O	0.130372	0.000000	-2.715384	2.730371	0.149409	0.000000	2.732843	0.118742	0.000000	0.152219	0.000000	-2.749783

Table S9 Coordinates of $Ru_3(CO)_{10}$ (**10-1**)

	MPW1PW91/SDD			MPW1PW91/LANL2DZ			BP86/SDD			BP86/LANL2DZ		
Ru	0.486943	1.542492	0.257078	0.145103	1.641515	0.271127	0.734004	1.454206	0.250564	0.599699	1.531759	0.251506
Ru	-1.499062	-0.339520	-0.071334	-1.398116	-0.673370	-0.081339	-1.551865	-0.092065	-0.058977	-1.540416	-0.225816	-0.055509
Ru	1.103827	-1.180004	-0.138834	1.379394	-0.881036	-0.163937	0.857156	-1.366584	-0.144022	1.003168	-1.303168	-0.172437
C	0.046191	0.712920	-1.411515	-0.282249	0.734247	-1.400249	0.367447	0.590937	-1.436348	0.230268	0.626554	-1.441790
C	-0.161623	3.305799	-0.133312	-0.959541	3.197725	-0.085388	0.453749	3.290831	-0.210025	0.208091	3.354996	-0.230122
C	2.255092	2.179284	0.030606	1.710939	2.636825	-0.128607	2.610984	1.811014	0.237495	2.464098	1.984098	0.219236
C	-1.605188	1.194924	1.181915	-1.749716	0.703417	1.318858	-1.375059	1.566487	1.061449	-1.516005	1.483361	1.057281
C	-2.926401	0.213225	-1.219478	-3.079800	-0.384601	-1.011709	-2.801880	0.597493	-1.313522	-2.897628	0.328933	-1.281560
C	-2.598111	-1.351199	1.119792	-1.969806	-2.031843	1.176111	-2.938568	-0.762931	1.049288	-2.821525	-1.036714	1.112585
C	-0.985069	-2.046923	-0.908580	-0.652545	-2.086223	-1.214918	-1.242710	-1.992350	-0.698806	-1.070896	-2.068475	-0.767579
C	1.238721	-0.203375	1.466105	1.302544	0.150131	1.422261	1.101180	-0.408045	1.506221	1.002939	-0.326090	1.500584
C	1.355729	-2.973533	0.367955	1.817652	-2.648562	0.328079	0.983895	-3.158946	0.447262	1.263731	-3.098223	0.386736
C	2.938704	-1.063463	-0.596966	3.212178	-0.499415	-0.491276	2.666163	-1.500843	-0.747569	2.871156	-1.216306	-0.616790
O	0.222524	0.711590	-2.577828	-0.114316	0.820973	-2.563930	0.481180	0.587652	-2.626289	0.385092	0.633197	-2.626091
O	-0.509473	4.362231	-0.418013	-1.576500	4.131491	-0.336747	0.325780	4.405205	-0.536291	0.013398	4.455209	-0.569025
O	3.320671	2.574179	-0.149409	2.653583	3.226929	-0.422578	3.752490	2.058655	0.194284	3.590375	2.292289	0.169840
O	-2.067783	1.850206	2.022567	-2.240012	1.209635	2.238950	-1.802956	2.340407	1.847578	-2.041296	2.220193	1.816201
O	-3.780425	0.496952	-1.932729	-4.063870	-0.277243	-1.591853	-3.565316	0.976728	-2.112783	-3.723279	0.618067	-2.055284
O	-3.275433	-1.944382	1.831203	-2.321883	-2.837450	1.912613	-3.797062	-1.149711	1.739547	-3.617366	-1.506831	1.824679
O	-1.133458	-3.056379	-1.464407	-0.469312	-2.963544	-1.943422	-1.675967	-3.010643	-1.119716	-1.398097	-3.096934	-1.249581
O	1.456214	-0.055451	2.608090	1.500954	0.333976	2.564378	1.327749	-0.352974	2.671812	1.180467	-0.281390	2.675208
O	1.540491	-4.036486	0.772290	2.101608	-3.683361	0.750739	1.095266	-4.246758	0.863592	1.454583	-4.176717	0.798692
O	4.053746	-1.004534	-0.872166	4.322407	-0.269278	-0.685202	3.773815	-1.609359	-1.104930	4.011968	-1.196453	-0.868157

Table S10 Coordinates of $Ru_3(CO)_{10}$ (**10-2**)

	MPW1PW91/SDD			MPW1PW91/LANL2DZ			BP86/SDD			BP86/LANL2DZ		
Ru	0.000000	0.000000	1.522580	0.000000	0.000000	1.496823	0.000000	0.000000	1.551999	0.000000	0.000000	1.552529
Ru	-1.380189	0.318858	-0.792694	-1.406703	0.350110	-0.806164	-1.402114	0.271111	-0.797139	-1.424226	0.271475	-0.804764
Ru	1.380189	-0.318858	-0.792694	1.406703	-0.350110	-0.806164	1.402114	-0.271111	-0.797139	1.424226	-0.271475	-0.804764
C	1.987462	0.148605	1.333164	2.017570	0.125141	1.309910	1.997062	0.216651	1.321895	2.016461	0.212162	1.319620
C	0.166208	-1.360620	2.825719	0.130667	-1.382387	2.811520	0.212743	-1.347197	2.863898	0.201947	-1.354367	2.876139
C	-0.166208	1.360620	2.825719	-0.130667	1.382387	2.811520	-0.212743	1.347197	2.863898	-0.201947	1.354367	2.876139
C	0.000000	1.594601	-0.611578	0.000000	1.586394	-0.414759	0.000000	1.579100	-0.675837	0.000000	1.573982	-0.600710
C	-2.933162	1.405092	-0.758107	-2.961708	1.447538	-0.801673	-2.952231	1.374035	-0.757203	-2.977779	1.384521	-0.787691
C	-1.606503	0.160246	-2.679897	-1.499322	0.331198	-2.719506	-1.696111	0.049689	-2.677073	-1.654760	0.083131	-2.707525
C	0.000000	-1.594601	-0.611578	0.000000	-1.586394	-0.414759	0.000000	-1.579100	-0.675837	0.000000	-1.573982	-0.600710
C	1.606503	-0.160246	-2.679897	1.499322	-0.331198	-2.719506	1.696111	-0.049689	-2.677073	1.654760	-0.083131	-2.707525
C	2.933162	-1.405092	-0.758107	2.961708	-1.447538	-0.801673	2.952231	-1.374035	-0.757203	2.977779	-1.384521	-0.787691
C	-1.987462	-0.148605	1.333164	-2.017570	-0.125141	1.309910	-1.997062	-0.216651	1.321895	-2.016461	-0.212162	1.319620
O	3.042850	0.350790	1.782331	3.054281	0.329013	1.795746	3.062870	0.475751	1.766204	3.073615	0.468388	1.781624
O	0.229796	-2.189324	3.618094	0.180781	-2.203686	3.610892	0.299978	-2.186196	3.672274	0.283452	-2.186561	3.691170
O	-0.229796	2.189324	3.618094	-0.180781	2.203686	3.610892	-0.299978	2.186196	3.672274	-0.283452	2.186561	3.691170
O	0.483845	2.657322	-0.721511	0.502837	2.640405	-0.538623	0.415509	2.690620	-0.784110	0.404870	2.688091	-0.716810
O	-3.839052	2.113939	-0.770156	-3.853450	2.173432	-0.825638	-3.875956	2.090977	-0.769993	-3.895337	2.108516	-0.812235
O	-1.761485	0.108874	-3.818016	-1.603275	0.365286	-3.863855	-1.896573	-0.042449	-3.824864	-1.821713	0.015052	-3.861877
O	-0.483845	-2.657322	-0.721511	-0.502837	-2.640405	-0.538623	-0.415509	-2.690620	-0.784110	-0.404870	-2.688091	-0.716810
O	1.761485	-0.108874	-3.818016	1.603275	-0.365286	-3.863855	1.896573	0.042449	-3.824864	1.821713	-0.015052	-3.861877
O	3.839052	-2.113939	-0.770156	3.853450	-2.173432	-0.825638	3.875956	-2.090977	-0.769993	3.895337	-2.108516	-0.812235
O	-3.042850	-0.350790	1.782331	-3.054281	-0.329013	1.795746	-3.062870	-0.475751	1.766204	-3.073615	-0.468388	1.781624

Table S11 Coordinates of $Ru_3(CO)_{10}$ (**10-3**)

	MPW1PW91/SDD			MPW1PW91/LANL2DZ			BP86/SDD			BP86/LANL2DZ		
Ru	-0.746400	0.009377	1.339929	-0.748824	0.005697	1.344241	-0.747561	0.012509	1.363557	-0.751617	0.008596	1.369309
Ru	-0.746400	0.009377	-1.339929	-0.748824	0.005697	-1.344241	-0.747561	0.012509	-1.363557	-0.751617	0.008596	-1.369309
Ru	1.659908	0.262766	0.000000	1.670035	0.274010	0.000000	1.681841	0.231711	0.000000	1.693896	0.244209	0.000000
C	0.000003	1.513489	0.000000	-0.003546	1.533987	0.000000	0.031885	1.511808	0.000000	0.030629	1.529393	0.000000
C	-1.399455	1.375850	2.444593	-1.416823	1.373165	2.457423	-1.469800	1.373440	2.435944	-1.475589	1.370870	2.456364
C	0.187720	-0.705796	2.838263	0.213855	-0.695059	2.850087	0.196021	-0.655462	2.888474	0.216382	-0.656422	2.896427
C	-2.395127	-0.983022	1.446158	-2.412521	-0.997561	1.445542	-2.383392	-1.004871	1.454506	-2.406892	-1.007629	1.451642
C	-1.399455	1.375850	-2.444593	-1.416823	1.373165	-2.457423	-1.469800	1.373440	-2.435944	-1.475589	1.370870	-2.456364
C	-2.395127	-0.983022	-1.446158	-2.412521	-0.997561	-1.445542	-2.383392	-1.004871	-1.454506	-2.406892	-1.007629	-1.451642
C	0.187720	-0.705796	-2.838263	0.213855	-0.695059	-2.850087	0.196021	-0.655462	-2.888474	0.216382	-0.656422	-2.896427
C	0.793199	-1.419919	0.000000	0.762766	-1.413502	0.000000	0.800827	-1.459382	0.000000	0.774514	-1.451369	0.000000
C	2.939215	0.035031	-1.402982	2.953535	0.028121	-1.408771	2.971259	0.051257	-1.410624	2.984646	0.044918	-1.418998
C	2.939215	0.035031	1.402982	2.953535	0.028121	1.408771	2.971259	0.051257	1.410624	2.984646	0.044918	1.418998
O	0.107318	2.697363	0.000000	0.077209	2.715639	0.000000	0.111340	2.717083	0.000000	0.088553	2.731716	0.000000
O	-1.811772	2.235812	3.085729	-1.834051	2.230022	3.098381	-1.927355	2.242906	3.069234	-1.930349	2.238061	3.093760
O	0.724831	-1.172979	3.740880	0.758643	-1.154190	3.751453	0.731216	-1.106268	3.824505	0.757591	-1.106960	3.828456
O	-3.361174	-1.583627	1.608887	-3.374983	-1.602018	1.611275	-3.352376	-1.637129	1.617967	-3.377047	-1.636238	1.618941
O	-1.811772	2.235812	-3.085729	-1.834051	2.230022	-3.098381	-1.927355	2.242906	-3.069234	-1.930349	2.238061	-3.093760
O	-3.361174	-1.583627	-1.608887	-3.374983	-1.602018	-1.611275	-3.352376	-1.637129	-1.617967	-3.377047	-1.636238	-1.618941
O	0.724831	-1.172979	-3.740880	0.758643	-1.154190	-3.751453	0.731216	-1.106268	-3.824505	0.757591	-1.106960	-3.828456
O	0.860917	-2.594074	0.000000	0.860109	-2.585595	0.000000	0.830684	-2.651059	0.000000	0.831099	-2.641929	0.000000
O	3.707736	-0.131666	-2.242951	3.719429	-0.150378	-2.248343	3.766193	-0.081461	-2.258830	3.774819	-0.101670	-2.268875
O	3.707736	-0.131666	2.242951	3.719429	-0.150378	2.248343	3.766193	-0.081461	2.258830	3.774819	-0.101670	2.268875

Table S12 Coordinates of $Ru_3(CO)_{10}$ (**10-4**)

	MPW1PW91/SDD			MPW1PW91/LANL2DZ			BP86/SDD			BP86/LANL2DZ		
Ru	0.000000	1.402670	-0.804171	0.000000	1.417604	-0.820689	0.000000	1.419615	-0.803838	0.000000	1.436425	-0.819180
Ru	0.000000	0.000000	1.535627	0.000000	0.000000	1.552301	0.000000	0.000000	1.547826	0.000000	0.000000	1.565228
Ru	0.000000	-1.402670	-0.804171	0.000000	-1.417604	-0.820689	0.000000	-1.419615	-0.803838	0.000000	-1.436425	-0.819180
C	0.000000	0.000000	-2.398502	0.000000	0.000000	-2.420179	0.000000	0.000000	-2.393608	0.000000	0.000000	-2.412246
C	-0.082816	-2.101735	1.174970	-0.071854	-2.112705	1.184229	-0.133833	-2.118041	1.175609	-0.129718	-2.129998	1.185673
C	0.082816	2.101735	1.174970	0.071854	2.112705	1.184229	0.133833	2.118041	1.175609	0.129718	2.129998	1.185673
C	0.762295	2.822261	-1.756663	0.628383	2.912249	-1.794910	0.872719	2.768366	-1.761196	0.727611	2.870975	-1.807979
C	-1.593152	2.183079	-1.236763	-1.670799	2.077264	-1.182262	-1.531551	2.314143	-1.278773	-1.623966	2.208014	-1.215352
C	-1.941406	0.107356	1.511558	-1.950726	0.098326	1.506416	-1.949626	0.147752	1.525846	-1.957420	0.146659	1.516319
C	1.941406	-0.107356	1.511558	1.950726	-0.098326	1.506416	1.949626	-0.147752	1.525846	1.957420	-0.146659	1.516319
C	-0.762295	-2.822261	-1.756663	-0.628383	-2.912249	-1.794910	-0.872719	-2.768366	-1.761196	-0.727611	-2.870975	-1.807979
C	1.593152	-2.183079	-1.236763	1.670799	-2.077264	-1.182262	1.531551	-2.314143	-1.278773	1.623966	-2.208014	-1.215352
C	0.000000	0.000000	3.463029	0.000000	0.000000	3.488770	0.000000	0.000000	3.485633	0.000000	0.000000	3.510303
O	0.000000	0.000000	-3.567357	0.000000	0.000000	-3.587572	0.000000	0.000000	-3.581571	0.000000	0.000000	-3.598593
O	-0.120157	-3.099554	1.783820	-0.086236	-3.112613	1.787019	-0.213897	-3.123980	1.801485	-0.186019	-3.137769	1.807470
O	0.120157	3.099554	1.783820	0.086236	3.112613	1.787019	0.213897	3.123980	1.801485	0.186019	3.137769	1.807470
O	1.296588	3.671565	-2.323399	1.074742	3.802829	-2.372709	1.498289	3.579263	-2.331900	1.260391	3.731949	-2.397777
O	-2.623900	2.641049	-1.484471	-2.740376	2.460174	-1.387295	-2.541834	2.844938	-1.556075	-2.680251	2.664891	-1.447485
O	-3.086693	0.171640	1.532953	-3.096473	0.156896	1.507238	-3.111824	0.233016	1.559879	-3.119912	0.233913	1.528638
O	3.086693	-0.171640	1.532953	3.096473	-0.156896	1.507238	3.111824	-0.233016	1.559879	3.119912	-0.233913	1.528638
O	-1.296588	-3.671565	-2.323399	-1.074742	-3.802829	-2.372709	-1.498289	-3.579263	-2.331900	-1.260391	-3.731949	-2.397777
O	2.623900	-2.641049	-1.484471	2.740376	-2.460174	-1.387295	2.541834	-2.844938	-1.556075	2.680251	-2.664891	-1.447485
O	0.000000	0.000000	4.611433	0.000000	0.000000	4.637332	0.000000	0.000000	4.652727	0.000000	0.000000	4.677598

Table S13 Coordinates of $Ru_3(CO)_{10}$ (**10-5**)

	MPW1PW91/SDD			MPW1PW91/LANL2DZ			BP86/SDD			BP86/LANL2DZ		
Ru	0.000000	1.550540	-0.012871	0.000000	1.553067	-0.011643	0.000000	1.575235	-0.006286	0.000000	1.580794	-0.004888
Ru	1.342807	-0.775270	-0.012871	1.344995	-0.776533	-0.011643	1.364193	-0.787617	-0.006286	1.369008	-0.790397	-0.004888
Ru	-1.342807	-0.775270	-0.012871	-1.344995	-0.776533	-0.011643	-1.364193	-0.787617	-0.006286	-1.369008	-0.790397	-0.004888
C	0.000000	0.000000	1.476651	0.000000	0.000000	1.502011	0.000000	0.000000	1.469201	0.000000	0.000000	1.489861
C	0.000000	2.878568	1.325981	0.000000	2.904022	1.323097	0.000000	2.919759	1.322667	0.000000	2.947274	1.318121
C	-1.427201	2.434067	-0.916426	-1.444617	2.433673	-0.918627	-1.436205	2.450508	-0.918692	-1.454318	2.449986	-0.919741
C	1.427201	2.434067	-0.916426	1.444617	2.433673	-0.918627	1.436205	2.450508	-0.918692	1.454318	2.449986	-0.919741
C	2.492913	-1.439284	1.325981	2.514957	-1.452011	1.323097	2.528586	-1.459880	1.322667	2.552414	-1.473637	1.318121
C	2.821564	0.018959	-0.916426	2.829931	0.034239	-0.918627	2.840305	0.018536	-0.918692	2.848909	0.034483	-0.919741
C	1.394363	-2.453025	-0.916426	1.385314	-2.467911	-0.918627	1.404100	-2.469044	-0.918692	1.394591	-2.484469	-0.919741
C	-2.492913	-1.439284	1.325981	-2.514957	-1.452011	1.323097	-2.528586	-1.459880	1.322667	-2.552414	-1.473637	1.318121
C	-1.394363	-2.453025	-0.916426	-1.385314	-2.467911	-0.918627	-1.404100	-2.469044	-0.918692	-1.394591	-2.484469	-0.919741
C	-2.821564	0.018959	-0.916426	-2.829931	0.034239	-0.918627	-2.840305	0.018536	-0.918692	-2.848909	0.034483	-0.919741
O	0.000000	0.000000	2.659867	0.000000	0.000000	2.680771	0.000000	0.000000	2.673793	0.000000	0.000000	2.689926
O	0.000000	3.648139	2.179549	0.000000	3.675871	2.173865	0.000000	3.710673	2.183292	0.000000	3.740369	2.176102
O	-2.209819	3.051268	-1.492195	-2.221373	3.055503	-1.496654	-2.226403	3.078639	-1.510623	-2.238820	3.082830	-1.513652
O	2.209819	3.051268	-1.492195	2.221373	3.055503	-1.496654	2.226403	3.078639	-1.510623	2.238820	3.082830	-1.513652
O	3.159381	-1.824069	2.179549	3.183398	-1.837935	2.173865	3.213537	-1.855336	2.183292	3.239254	-1.870184	2.176102
O	3.747386	0.388125	-1.492195	3.756830	0.396014	-1.496654	3.779381	0.388801	-1.510623	3.789219	0.397460	-1.513652
O	1.537566	-3.439394	-1.492195	1.535457	-3.451517	-1.496654	1.552979	-3.467441	-1.510623	1.550399	-3.480290	-1.513652
O	-3.159381	-1.824069	2.179549	-3.183398	-1.837935	2.173865	-3.213537	-1.855336	2.183292	-3.239254	-1.870184	2.176102
O	-1.537566	-3.439394	-1.492195	-1.535457	-3.451517	-1.496654	-1.552979	-3.467441	-1.510623	-1.550399	-3.480290	-1.513652
O	-3.747386	0.388125	-1.492195	-3.756830	0.396014	-1.496654	-3.779381	0.388801	-1.510623	-3.789219	0.397460	-1.513652

Table S14 Coordinates of $Ru_3(CO)_9$ (**9-1**)

	MPW1PW91/SDD			MPW1PW91/LANL2DZ			BP86/SDD			BP86/LANL2DZ		
Ru	1.208351	-0.786204	-0.158835	1.217173	-0.800780	-0.163871	1.193432	-0.854085	-0.152059	1.204528	-0.863803	-0.156689
Ru	-0.056853	1.546965	-0.192098	-0.050747	1.551979	-0.220445	-0.021684	1.565743	-0.177138	-0.020169	1.574408	-0.197826
Ru	-1.519896	-0.786613	0.261846	-1.533281	-0.784790	0.283452	-1.510266	-0.773559	0.231366	-1.526390	-0.774656	0.248501
C	0.310683	-1.407481	1.402301	0.295428	-1.324703	1.446664	0.265559	-1.343242	1.472222	0.256481	-1.278429	1.500681
C	-2.055170	0.048990	1.922680	-2.089227	0.111488	1.917750	-2.232289	0.002472	1.849267	-2.253310	0.051806	1.850188
C	2.936850	-0.194717	0.266842	2.954013	-0.187956	0.239477	2.929086	-0.206004	0.242145	2.948971	-0.204286	0.218048
C	1.924103	-2.488828	-0.503167	1.926228	-2.537621	-0.405725	1.925083	-2.578554	-0.397834	1.924680	-2.613782	-0.322056
C	-0.412042	1.355365	-2.088930	-0.418855	1.298447	-2.117325	-0.376683	1.433918	-2.084114	-0.375841	1.383579	-2.108275
C	1.276382	2.772873	-0.578983	1.298939	2.762686	-0.646236	1.333191	2.799170	-0.515762	1.347875	2.798835	-0.566655
C	0.441485	1.677210	1.676178	0.442863	1.732408	1.658913	0.341082	1.743710	1.726745	0.349583	1.776685	1.714555
C	-0.922997	-1.480384	-1.449935	-0.914560	-1.545141	-1.408140	-0.726102	-1.439299	-1.452133	-0.732190	-1.485908	-1.426805
C	-3.151778	-0.228067	-0.530820	-3.164922	-0.244503	-0.554129	-3.111898	-0.320081	-0.699135	-3.130153	-0.330185	-0.706612
O	0.368381	-1.909418	2.464678	0.397854	-1.754141	2.535681	0.347421	-1.771547	2.582961	0.371583	-1.653182	2.626235
O	-2.426055	0.541835	2.890843	-2.465209	0.635904	2.866542	-2.718589	0.468565	2.802930	-2.736589	0.546991	2.789948
O	3.976284	0.145078	0.634786	3.990608	0.173840	0.592501	3.984202	0.174876	0.580640	4.003689	0.188029	0.542853
O	2.369924	-3.523690	-0.749570	2.364538	-3.589290	-0.581463	2.391317	-3.640125	-0.572739	2.381376	-3.686736	-0.439694
O	-0.596563	1.308821	-3.221471	-0.615526	1.206240	-3.244623	-0.582481	1.453546	-3.232671	-0.580282	1.356565	-3.256541
O	2.142570	3.494551	-0.835565	2.170723	3.468073	-0.925272	2.219857	3.536678	-0.742002	2.240014	3.522743	-0.811224
O	0.788318	1.815578	2.761401	0.780825	1.894100	2.743015	0.590316	1.938518	2.849034	0.601347	1.977857	2.834567
O	-0.733603	-1.902584	-2.507779	-0.725885	-2.003727	-2.450204	-0.547375	-1.844325	-2.544123	-0.557232	-1.916965	-2.508203
O	-4.123705	0.130794	-1.034472	-4.127659	0.104926	-1.079863	-4.083093	-0.044797	-1.292004	-4.094813	-0.056763	-1.309667

Table S15 Coordinates of $Ru_3(CO)_9$ (**9-2**)

	MPW1PW91/SDD			MPW1PW91/LANL2DZ			BP86/SDD			BP86/LANL2DZ		
Ru	1.066113	-0.900443	0.000000	-1.034092	-0.963397	0.000000	1.117482	-0.901616	0.000000	1.087566	-0.969406	0.000000
Ru	-1.713341	-0.725239	0.000000	1.774899	-0.652479	0.000000	-1.706250	-0.748479	0.000000	-1.771266	-0.674087	0.000000
Ru	-0.047901	1.527079	0.000000	-0.020067	1.528722	0.000000	-0.065969	1.537972	0.000000	0.003054	1.540187	0.000000
C	-0.473632	-0.721569	1.492822	0.511595	-0.669462	-1.492606	-0.460909	-0.771298	1.504075	-0.504461	-0.718452	1.502777
C	-0.473632	-0.721569	-1.492822	0.511595	-0.669462	1.492606	-0.460909	-0.771298	-1.504075	-0.504461	-0.718452	-1.502777
C	-2.299212	-2.548764	0.000000	2.368919	-2.488383	0.000000	-2.432894	-2.528815	0.000000	-2.519922	-2.459813	0.000000
C	2.110034	-1.819753	-1.303378	-2.047766	-1.923484	1.314669	2.205976	-1.781410	-1.301053	2.144638	-1.890467	-1.312212
C	2.110034	-1.819753	1.303378	-2.047766	-1.923484	-1.314669	2.205976	-1.781410	1.301053	2.144638	-1.890467	1.312212
C	-2.001838	1.489152	0.000000	1.959098	1.569747	0.000000	-2.037894	1.426981	0.000000	-1.995001	1.521531	0.000000
C	0.288237	2.830063	1.288277	-0.398778	2.830767	-1.291420	0.222845	2.851548	1.297091	0.344366	2.851854	1.298777
C	2.028441	0.826473	0.000000	-2.071901	0.738594	0.000000	2.015805	0.888937	0.000000	2.061794	0.795375	0.000000
C	0.288237	2.830063	-1.288277	-0.398778	2.830767	1.291420	0.222845	2.851548	-1.297091	0.344366	2.851854	-1.298777
O	-0.603834	-0.789420	2.663682	0.642004	-0.729494	-2.662637	-0.557279	-0.869666	2.693697	-0.600042	-0.812784	2.691639
O	-0.603834	-0.789420	-2.663682	0.642004	-0.729494	2.662637	-0.557279	-0.869666	-2.693697	-0.600042	-0.812784	-2.691639
O	-2.606180	-3.656391	0.000000	2.672896	-3.596291	0.000000	-2.854671	-3.619833	0.000000	-2.944514	-3.549031	0.000000
O	2.758554	-2.375265	-2.073316	-2.677759	-2.498847	2.084679	2.890186	-2.323905	-2.078110	2.808817	-2.453646	-2.091333
O	2.758554	-2.375265	2.073316	-2.677759	-2.498847	-2.084679	2.890186	-2.323905	2.078110	2.808817	-2.453646	2.091333
O	-3.140733	1.753750	0.000000	3.062484	1.950810	0.000000	-3.205500	1.660910	0.000000	-3.128286	1.878025	0.000000
O	0.490105	3.604054	2.114160	-0.627001	3.599164	-2.114874	0.393364	3.644066	2.140423	0.547893	3.639373	2.138717
O	3.097967	1.307964	0.000000	-3.163604	1.161480	0.000000	3.098052	1.386026	0.000000	3.166047	1.236082	0.000000
O	0.490105	3.604054	-2.114160	-0.627001	3.599164	2.114874	0.393364	3.644066	-2.140423	0.547893	3.639373	-2.138717

Table S16 Coordinates of $Ru_3(CO)_9$ (**9-3**)

	MPW1PW91/SDD			MPW1PW91/LANL2DZ			BP86/SDD			BP86/LANL2DZ		
Ru	0.616055	1.453298	-0.159400	0.607634	1.471924	-0.154240	0.604095	1.462604	-0.119504	0.591439	1.487341	-0.125036
Ru	0.950566	-1.260168	-0.159400	0.970907	-1.262188	-0.154240	0.964605	-1.254464	-0.119504	0.992356	-1.255871	-0.125036
Ru	-1.566621	-0.193130	-0.159400	-1.578541	-0.209736	-0.154240	-1.568700	-0.208141	-0.119504	-1.583795	-0.231470	-0.125036
C	1.625192	0.698102	1.224524	1.631984	0.655570	1.218189	1.669267	0.679642	1.244127	1.665743	0.644550	1.229687
C	0.000000	3.265239	-0.043477	0.000000	3.293009	-0.048348	0.000000	3.277618	-0.033956	0.000000	3.308932	-0.017091
C	2.200719	1.977977	-1.028513	2.202313	1.996590	-1.032142	2.139465	1.947674	-1.107803	2.141448	1.981730	-1.109730
C	-0.208022	-1.756508	1.224524	-0.248252	-1.741125	1.218189	-0.246046	-1.785449	1.244127	-0.274675	-1.764851	1.229687
C	2.827780	-1.632620	-0.043477	2.851830	-1.646505	-0.048348	2.838500	-1.638809	-0.033956	2.865619	-1.654466	-0.017091
C	0.612619	-2.894867	-1.028513	0.627941	-2.905554	-1.032142	0.617003	-2.826668	-1.107803	0.645505	-2.845413	-1.109730
C	-1.417169	1.058406	1.224524	-1.383733	1.085555	1.218189	-1.423221	1.105806	1.244127	-1.391068	1.120301	1.229687
C	-2.827780	-1.632620	-0.043477	-2.851830	-1.646505	-0.048348	-2.838500	-1.638809	-0.033956	-2.865619	-1.654466	-0.017091
C	-2.813338	0.916890	-1.028513	-2.830254	0.908964	-1.032142	-2.756467	0.878994	-1.107803	-2.786953	0.863683	-1.109730
O	2.237776	0.625694	2.212362	2.247632	0.608984	2.205350	2.320178	0.645322	2.231685	2.313612	0.639731	2.219655
O	-0.275299	4.364034	0.162005	-0.273157	4.392660	0.153537	-0.270938	4.404513	0.136355	-0.264618	4.434430	0.169167
O	3.147903	2.273316	-1.612070	3.149893	2.290836	-1.613839	3.051920	2.220709	-1.787541	3.059033	2.261199	-1.778272
O	-0.577021	-2.250818	2.212362	-0.596421	-2.250998	2.205350	-0.601223	-2.331994	2.231685	-0.602783	-2.323512	2.219655
O	3.917014	-1.943601	0.162005	3.940734	-1.959769	0.153537	3.949889	-1.967618	0.136355	3.972638	-1.988049	0.169167
O	0.394798	-3.862821	-1.612070	0.408976	-3.873306	-1.613839	0.397230	-3.753395	-1.787541	0.428739	-3.779800	-1.778272
O	-1.660755	1.625124	2.212362	-1.651211	1.642015	2.205350	-1.718954	1.686672	2.231685	-1.710829	1.683782	2.219655
O	-3.641715	-2.420433	0.162005	-3.667577	-2.432891	0.153537	-3.678952	-2.436896	0.136355	-3.708020	-2.446380	0.169167
O	-3.542700	1.589506	-1.612070	-3.558869	1.582470	-1.613839	-3.449150	1.532686	-1.787541	-3.487772	1.518601	-1.778272

Table S17 Coordinates of $Ru_3(CO)_9$ (**9-4**)

	MPW1PW91/SDD			MPW1PW91/LANL2DZ			BP86/SDD			BP86/LANL2DZ		
Ru	0.000000	1.592245	0.102868	0.000000	1.607226	0.103267	0.000000	1.601515	0.101536	0.000000	1.617996	0.104119
Ru	1.378925	-0.796123	0.102868	1.391899	-0.803613	0.103267	1.386953	-0.800758	0.101536	1.401226	-0.808998	0.104119
Ru	-1.378925	-0.796123	0.102868	-1.391899	-0.803613	0.103267	-1.386953	-0.800758	0.101536	-1.401226	-0.808998	0.104119
C	-0.685928	1.599218	-1.730399	-0.688189	1.610695	-1.740493	-0.771068	1.591510	-1.702144	-0.767866	1.599721	-1.711068
C	0.692637	1.565568	1.887326	0.695177	1.574974	1.900459	0.691617	1.611675	1.897581	0.704570	1.613996	1.907898
C	1.262960	2.892545	-0.301032	1.281505	2.902264	-0.303743	1.214952	2.953981	-0.332998	1.233200	2.964263	-0.335159
C	1.009503	-1.382625	1.887326	1.016379	-1.389528	1.900459	1.049943	-1.404795	1.897581	1.045477	-1.417174	1.907898
C	1.727928	-0.205578	-1.730399	1.738997	-0.209358	-1.740493	1.763822	-0.127990	-1.702144	1.769332	-0.134869	-1.711068
C	1.873538	-2.540028	-0.301032	1.872682	-2.560947	-0.303743	1.950747	-2.529170	-0.332998	1.950527	-2.550114	-0.335159
C	-1.702140	-0.182943	1.887326	-1.711556	-0.185446	1.900459	-1.741560	-0.206880	1.897581	-1.750047	-0.196823	1.907898
C	-1.042000	-1.393640	-1.730399	-1.050808	-1.401337	-1.740493	-0.992754	-1.463520	-1.702144	-1.001466	-1.464852	-1.711068
C	-3.136498	-0.352517	-0.301032	-3.154186	-0.341316	-0.303743	-3.165699	-0.424811	-0.332998	-3.183727	-0.414149	-0.335159
O	-1.096906	1.681621	-2.798991	-1.097845	1.683846	-2.809831	-1.245169	1.690050	-2.764157	-1.233434	1.685840	-2.777451
O	1.134055	1.666146	2.946449	1.133860	1.669607	2.960477	1.124814	1.744874	2.976827	1.144874	1.735887	2.984862
O	2.068683	3.664773	-0.605155	2.096215	3.662937	-0.610781	1.990943	3.770783	-0.667949	2.019196	3.768067	-0.676320
O	0.875898	-1.815193	2.946449	0.878992	-1.816755	2.960477	0.948699	-1.846554	2.976827	0.930885	-1.859434	2.984862
O	2.004779	0.109138	-2.798991	2.007176	0.108839	-2.809831	2.086210	0.233323	-2.764157	2.076698	0.225265	-2.777451
O	2.139445	-3.623919	-0.605155	2.124089	-3.646844	-0.610781	2.270122	-3.609598	-0.667949	2.253644	-3.632708	-0.676320
O	-2.009952	0.149047	2.946449	-2.012852	0.147148	2.960477	-2.073512	0.101680	2.976827	-2.075760	0.123547	2.984862
O	-0.907874	-1.790759	-2.798991	-0.909331	-1.792685	-2.809831	-0.841042	-1.923372	-2.764157	-0.843263	-1.911106	-2.777451
O	-4.208128	-0.040855	-0.605155	-4.220304	-0.016093	-0.610781	-4.261065	-0.161184	-0.667949	-4.272839	-0.135359	-0.676320

Table S18 Harmonic frequencies (cm^{-1}) and IR intensities (KM/Mole) of $Ru_3(CO)_{12}$ (**12-1**)

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
36(0), 37(0), 37(0), 49(0), 49(0), 52(0), 71(0), 71(0), 78(0), 78(0), 80(0), 87(1), 90(0), 92(0), 92(0), 100(0), 101(0), 101(0), 113(0), 113(0), 118(2), 118(2), 132(0), 135(0), 153(1), 153(1), 191(0), 381(1), 381(1), 394(0), 400(1), 400(1), 408(6), 413(2), 413(2), 417(0), 447(1), 447(1), 455(5), 457(4), 457(4), 460(0), 465(3), 465(3), 478(78), 482(0), 482(0), 486(0), 496(27), 496(27), 508(0), 536(18), 536(18), 539(0), 547(129), 568(2), 568(2), 578(12), 602(284), 602(284), 615(194), 615(194), 622(0), 2089(10), 2089(10), 2104(4), 2110(262), 2110(262), 2120(81), 2120(81), 2129(3115), 2132(0), 2158(2554), 2158(2554), 2218(0)	34(0), 34(0), 35(0), 48(0), 48(0), 53(0), 69(0), 69(0), 76(0), 76(0), 77(0), 84(0), 87(0), 89(0), 89(0), 97(0), 99(0), 99(0), 111(0), 111(0), 117(2), 117(2), 130(0), 133(0), 150(1), 150(1), 187(0), 367(1), 367(1), 381(0), 386(1), 386(1), 393(7), 398(3), 398(3), 404(0), 435(0), 435(0), 438(5), 443(1), 443(1), 450(6), 450(6), 451(0), 462(85), 466(0), 466(0), 470(0), 479(30), 479(30), 495(0), 522(15), 522(15), 524(0), 533(107), 551(1), 551(1), 562(5), 589(330), 589(330), 599(114), 599(114), 603(0), 2092(15), 2092(15), 2108(0), 2113(190), 2113(190), 2124(81), 2124(81), 2130(3069), 2135(0), 2160(2526), 2160(2526), 2217(0)	34(0), 34(0), 37(0), 47(0), 47(0), 52(0), 67(0), 67(0), 75(0), 75(0), 76(0), 82(0), 86(0), 86(0), 86(0), 94(0), 94(0), 95(0), 105(0), 105(0), 112(2), 112(2), 120(0), 123(0), 141(0), 141(0), 175(0), 357(1), 357(1), 369(0), 375(1), 375(1), 387(1), 389(3), 389(3), 394(1), 432(1), 432(1), 443(3), 443(3), 444(0), 446(0), 452(5), 452(5), 457(62), 467(1), 467(1), 475(0), 479(0), 480(10), 480(10), 505(15), 505(15), 507(0), 519(117), 536(1), 536(1), 547(2), 572(247), 572(247), 584(159), 584(159), 587(0), 1968(7), 1968(7), 1981(9), 1989(396), 1989(396), 1997(34), 1997(34), 2005(2594), 2008(0), 2036(1950), 2036(1950), 2088(0)	31(0), 31(0), 36(0), 46(0), 46(0), 52(0), 65(0), 65(0), 73(0), 73(0), 74(0), 79(0), 82(0), 83(0), 83(0), 92(0), 92(0), 93(0), 103(0), 103(0), 111(2), 111(2), 118(0), 121(0), 138(1), 138(1), 172(0), 344(1), 344(1), 356(0), 363(0), 363(0), 375(2), 375(2), 376(1), 380(0), 420(0), 420(0), 429(0), 430(1), 430(1), 438(0), 438(7), 438(7), 440(68), 453(1), 453(1), 462(0), 466(10), 466(10), 466(0), 491(13), 491(13), 494(0), 505(95), 520(1), 520(1), 533(0), 559(280), 559(280), 570(99), 570(99), 570(0), 1970(10), 1970(10), 1983(5), 1991(336), 1991(336), 1999(34), 1999(34), 2005(2550), 2009(0), 2036(1930), 2036(1930), 2086(0)

Table S19 Harmonic frequencies (cm^{-1}) and IR intensities (KM/Mole) of $Ru_3(CO)_{12}$ (**12-2**)

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
-15(0), 41(0), 42(0), 42(0), 53(0), 54(0), 69(0), 70(0), 75(0), 79(0), 82(0), 83(0), 87(0), 89(0), 90(0), 92(0), 95(0), 98(0), 98(0), 99(0), 110(0), 113(1), 156(1), 164(0), 172(0), 212(0), 224(6), 309(0), 373(7), 376(0), 396(0), 398(0), 405(0), 409(5), 414(13), 417(0), 420(25), 444(2), 446(60), 449(1), 450(10), 455(0), 460(7), 461(67), 467(15), 472(8), 472(0), 478(3), 490(15), 504(0), 504(10), 528(5), 533(0), 537(2), 555(155), 565(87), 566(0), 578(28), 593(96), 602(305), 607(509), 607(0), 613(78), 1935(880), 1984(250), 2109(75), 2112(4), 2121(624), 2126(0), 2127(167), 2136(129), 2141(2452), 2163(1969), 2164(2481), 2217(58)	-33(0), 40(0), 41(0), 41(0), 53(0), 53(0), 68(0), 70(0), 73(0), 76(0), 79(0), 80(0), 83(0), 87(0), 88(0), 89(0), 93(0), 96(0), 97(0), 99(1), 109(0), 113(0), 152(1), 160(0), 161(0), 204(0), 217(7), 298(0), 352(10), 358(1), 383(0), 385(0), 391(0), 395(6), 399(14), 403(0), 407(24), 430(51), 433(1), 436(25), 436(2), 443(0), 446(55), 450(5), 452(11), 454(11), 456(0), 460(4), 476(14), 488(10), 489(0), 513(5), 517(0), 524(0), 537(130), 548(81), 548(0), 564(21), 578(128), 585(267), 586(0), 592(436), 596(87), 1948(884), 1994(256), 2113(54), 2115(6), 2125(547), 2129(0), 2131(156), 2139(109), 2143(2386), 2165(1959), 2166(2438), 2216(58)	33(0), 39(0), 39(0), 40(0), 49(0), 50(0), 62(0), 65(0), 72(0), 75(0), 77(0), 79(0), 82(0), 85(0), 85(0), 86(0), 91(0), 92(0), 93(0), 94(0), 100(0), 102(0), 142(1), 150(0), 162(0), 194(0), 213(6), 291(0), 353(3), 357(0), 370(0), 374(0), 377(1), 388(1), 392(0), 392(17), 396(12), 419(1), 433(56), 437(4), 438(3), 441(0), 444(56), 449(6), 452(4), 455(2), 461(17), 468(1), 474(3), 475(0), 486(7), 500(0), 501(4), 505(0), 526(113), 536(14), 537(41), 547(36), 563(126), 574(417), 574(230), 576(0), 580(78), 1845(616), 1874(191), 1985(78), 1986(2), 1996(690), 2000(0), 2000(146), 2010(122), 2014(2068), 2038(2088), 2040(1399), 2084(69)	26(0), 37(0), 37(0), 38(0), 49(0), 50(0), 62(0), 65(0), 70(0), 72(0), 75(0), 76(0), 79(0), 83(0), 83(0), 83(0), 89(0), 90(0), 91(0), 93(1), 99(0), 102(0), 140(1), 147(0), 151(0), 188(0), 205(7), 282(0), 334(5), 339(1), 357(0), 362(0), 365(2), 375(1), 379(0), 381(16), 383(13), 409(3), 418(51), 424(3), 425(5), 428(57), 430(0), 437(2), 438(6), 443(0), 448(18), 454(1), 461(2), 462(0), 472(6), 486(0), 488(4), 494(0), 509(93), 521(13), 522(32), 535(36), 549(174), 557(0), 558(189), 559(338), 565(91), 1856(612), 1883(192), 1987(65), 1988(4), 1998(636), 2002(0), 2002(134), 2012(106), 2015(2016), 2038(2040), 2040(1384), 2083(69)

Table S20 Harmonic frequencies (cm^{-1}) and IR intensities (KM/Mole) of $Ru_3(CO)_{12}$ (**12-3**)

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
-14(0), 30(0), 40(0), 40(0), 41(0), 41(0), 72(0), 72(0), 73(0), 73(0), 80(0), 88(0), 89(0), 94(0), 97(0), 97(0), 103(1), 103(1), 118(0), 118(0), 123(0), 123(0), 150(1), 150(1), 156(0), 158(0), 186(0), 396(0), 396(0), 400(2), 400(2), 403(0), 409(0), 409(0), 411(0), 422(10), 445(0), 445(0), 451(0), 456(0), 458(4), 458(4), 471(0), 471(0), 473(107), 478(13), 478(13), 490(0), 497(45), 497(45), 521(0), 538(0), 540(0), 540(0), 575(0), 575(0), 577(88), 585(0), 605(89), 605(89), 630(362), 630(362), 631(0), 2097(0), 2097(0), 2099(0), 2114(20), 2114(20), 2117(485), 2117(485), 2140(3053), 2141(0), 2163(2377), 2163(2376), 2225(0)	-16(0), 30(0), 40(0), 40(0), 42(0), 42(0), 70(0), 70(0), 72(0), 72(0), 77(0), 85(0), 86(0), 92(0), 93(0), 93(0), 103(1), 103(1), 117(0), 117(0), 122(0), 122(0), 148(1), 148(1), 156(0), 158(0), 182(0), 382(0), 382(0), 387(2), 387(2), 392(0), 394(0), 394(0), 399(0), 407(8), 432(0), 433(1), 433(1), 442(4), 442(4), 447(0), 456(99), 460(0), 460(0), 462(12), 462(12), 474(0), 481(45), 481(45), 507(0), 523(0), 525(0), 525(0), 559(0), 559(0), 562(76), 575(0), 593(65), 593(65), 613(0), 614(350), 614(350), 2099(0), 2099(0), 2103(0), 2118(0), 2118(0), 2120(390), 2120(390), 2141(3002), 2144(0), 2164(2400), 2164(2400), 2224(0)	-14(0), 26(0), 34(0), 34(0), 36(0), 36(0), 67(0), 67(0), 69(0), 69(0), 73(0), 82(0), 84(0), 90(0), 90(0), 90(0), 97(1), 97(1), 108(0), 108(0), 114(0), 114(0), 137(1), 137(1), 143(0), 144(0), 170(0), 369(1), 369(1), 371(0), 371(0), 380(0), 383(0), 391(0), 391(0), 403(1), 429(1), 429(1), 442(0), 443(0), 447(10), 447(10), 451(87), 455(0), 455(0), 461(13), 461(13), 478(0), 484(18), 484(18), 493(0), 507(0), 507(0), 507(0), 541(72), 543(0), 543(0), 562(0), 573(56), 573(56), 594(0), 599(320), 599(320), 1975(0), 1975(0), 1978(0), 1991(30), 1991(30), 1995(558), 1995(558), 2014(2529), 2017(0), 2042(1779), 2042(1779), 2094(0)	-16(0), 30(0), 40(0), 40(0), 42(0), 42(0), 70(0), 70(0), 72(0), 72(0), 77(0), 85(0), 86(0), 92(0), 93(0), 93(0), 103(1), 103(1), 117(0), 117(0), 122(0), 122(0), 148(1), 148(1), 156(0), 158(0), 182(0), 382(0), 382(0), 387(2), 387(2), 392(0), 394(0), 394(0), 399(0), 407(8), 432(0), 433(1), 433(1), 442(4), 442(4), 447(0), 456(99), 460(0), 460(0), 462(12), 462(12), 474(0), 481(45), 481(45), 507(0), 523(0), 525(0), 525(0), 559(0), 559(0), 562(76), 575(0), 593(65), 593(65), 613(0), 614(350), 614(350), 2099(0), 2099(0), 2103(0), 2118(0), 2118(0), 2120(390), 2120(390), 2141(3002), 2144(0), 2164(2400), 2164(2400), 2224(0)

Table S21 Harmonic frequencies (cm^{-1}) and IR intensities (KM/Mole) of $Ru_3(CO)_{12}$ (**12-4**)

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
34(0), 53(0), 54(0), 54(0), 56(0), 56(0), 59(0), 67(0), 76(0), 76(0), 84(0), 84(0), 89(0), 89(0), 89(1), 94(0), 94(0), 109(0), 109(0), 112(0), 117(0), 129(0), 144(0), 144(0), 184(0), 209(8), 209(8), 339(0), 343(63), 343(63), 362(0), 384(0), 384(0), 402(0), 402(0), 405(171), 405(171), 412(61), 422(28), 431(0), 431(0), 444(0), 445(0), 445(0), 454(0), 486(8), 486(8), 490(0), 501(0), 509(3), 509(3), 510(0), 510(0), 521(55), 580(0), 580(0), 587(88), 615(213), 615(213), 622(0), 631(7), 631(7), 649(0), 1970(1330), 1970(1330), 2012(0), 2113(0), 2113(0), 2118(975), 2118(975), 2130(0), 2151(3186), 2177(975), 2177(975), 2228(0)	47(0), 52(0), 52(0), 56(0), 56(0), 56(0), 64(0), 66(0), 72(0), 72(0), 83(0), 83(0), 86(1), 88(0), 88(0), 90(0), 90(0), 105(0), 105(0), 112(0), 115(0), 138(0), 138(0), 138(0), 176(0), 201(7), 201(7), 324(51), 324(51), 337(0), 347(0), 370(0), 370(0), 391(0), 391(0), 394(150), 394(150), 401(45), 410(33), 421(0), 421(0), 436(0), 437(1), 437(1), 447(0), 474(7), 474(7), 483(0), 489(0), 495(0), 495(0), 500(4), 500(4), 506(50), 564(0), 564(0), 570(80), 604(199), 604(199), 611(0), 619(6), 619(6), 636(0), 1983(1253), 1983(1253), 2021(0), 2118(0), 2118(0), 2122(969), 2122(969), 2134(0), 2155(3082), 2179(941), 2179(941), 2229(0)	39(0), 47(0), 47(0), 53(0), 53(0), 58(0), 62(0), 71(0), 73(0), 73(0), 75(0), 75(0), 82(0), 82(0), 83(1), 87(0), 87(0), 99(0), 102(0), 102(0), 106(0), 132(0), 132(0), 139(0), 166(0), 201(3), 201(3), 319(0), 326(60), 326(60), 335(0), 359(0), 359(0), 388(123), 388(123), 393(0), 393(0), 397(0), 410(59), 419(0), 419(0), 424(0), 437(1), 437(1), 445(0), 461(0), 469(9), 469(9), 481(0), 481(0), 486(51), 494(0), 494(2), 494(2), 550(0), 550(0), 555(74), 589(170), 589(170), 589(0), 602(2), 602(2), 623(0), 1863(978), 1863(978), 1888(0), 1986(0), 1986(0), 1995(686), 1995(686), 2006(0), 2021(2694), 2052(943), 2052(943), 2096(0)	42(0), 46(0), 46(0), 53(0), 53(0), 55(0), 59(0), 68(0), 68(0), 74(0), 75(0), 75(0), 80(1), 81(0), 81(0), 84(0), 84(0), 99(0), 99(0), 100(0), 105(0), 128(0), 128(0), 143(0), 161(0), 193(3), 193(3), 307(49), 307(49), 318(0), 320(0), 346(0), 346(0), 377(107), 377(107), 381(0), 381(0), 386(0), 399(53), 408(0), 408(0), 417(0), 430(1), 430(1), 439(0), 455(0), 461(8), 461(8), 467(0), 467(0), 472(46), 485(0), 486(3), 486(3), 535(0), 535(0), 539(67), 579(162), 579(162), 579(0), 592(1), 592(1), 612(0), 1875(932), 1875(932), 1898(0), 1990(0), 1990(0), 1997(688), 1997(688), 2008(0), 2023(2607), 2053(907), 2053(907), 2097(0)

Table S22 Harmonic frequencies (cm^{-1}) and IR intensities (KM/Mole) of $Ru_3(CO)_{11}$ (**11-1**)

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
33(0), 38(0), 47(1), 49(0), 52(0), 58(0), 66(0), 69(0), 78(0), 81(0), 83(0), 85(0), 87(0), 91(0), 93(0), 97(0), 104(0), 105(0), 111(1), 112(0), 120(1), 143(2), 155(0), 165(1), 199(0), 326(19), 371(12), 388(10), 393(8), 394(3), 401(5), 406(4), 417(2), 430(1), 439(2), 444(32), 446(7), 455(6), 457(9), 464(13), 467(31), 476(8), 480(9), 483(7), 494(12), 496(18), 507(7), 524(5), 536(2), 553(131), 567(67), 571(18), 574(4), 581(83), 594(123), 597(179), 609(148), 612(109), 1991(508), 2064(417), 2095(346), 2104(184), 2108(188), 2117(99), 2133(2086), 2138(283), 2142(2415), 2157(1848), 2212(159)	31(0), 38(0), 47(1), 47(0), 51(0), 57(0), 64(0), 67(0), 76(0), 78(0), 80(0), 83(0), 85(0), 90(0), 90(0), 95(0), 102(0), 103(0), 109(1), 111(0), 119(1), 140(2), 149(0), 161(1), 193(0), 315(18), 360(11), 375(7), 378(3), 382(10), 389(6), 393(5), 403(3), 417(4), 423(7), 427(5), 435(21), 443(24), 446(10), 450(29), 453(3), 464(1), 466(12), 468(5), 480(18), 484(12), 493(5), 511(4), 521(3), 542(114), 551(47), 555(28), 561(17), 570(83), 582(47), 583(283), 592(95), 598(70), 1998(524), 2069(408), 2099(357), 2108(189), 2112(167), 2122(79), 2136(2099), 2143(168), 2146(2355), 2159(1803), 2213(155)	29(0), 33(0), 45(0), 48(0), 54(0), 54(0), 59(1), 63(0), 74(0), 76(0), 79(0), 80(0), 82(0), 85(0), 87(0), 91(0), 96(1), 98(0), 100(1), 104(0), 113(1), 143(1), 147(0), 156(2), 185(0), 297(18), 353(5), 368(14), 369(3), 371(5), 376(3), 380(2), 391(2), 414(3), 416(5), 426(22), 429(12), 441(15), 446(5), 449(14), 451(6), 457(1), 462(14), 468(21), 473(4), 479(4), 484(7), 497(5), 505(3), 525(90), 535(28), 541(15), 544(23), 546(99), 563(58), 565(171), 576(130), 580(101), 1861(402), 1936(398), 1974(207), 1983(259), 1986(83), 1993(126), 2008(1836), 2012(191), 2018(2088), 2033(1285), 2081(150)	26(0), 33(0), 44(0), 47(0), 52(0), 54(0), 58(0), 62(0), 72(0), 73(0), 76(0), 77(0), 80(0), 83(0), 85(0), 89(0), 93(0), 97(0), 99(1), 103(1), 112(1), 139(1), 142(0), 152(2), 179(0), 287(17), 343(4), 356(2), 357(6), 359(10), 366(4), 368(2), 378(3), 401(4), 403(7), 413(10), 415(22), 426(25), 435(5), 438(2), 438(6), 446(1), 450(16), 456(16), 464(5), 467(5), 473(5), 485(4), 493(5), 513(72), 520(20), 527(28), 531(41), 536(83), 550(74), 554(182), 561(104), 569(53), 1870(407), 1941(389), 1978(207), 1985(273), 1989(73), 1996(113), 2009(1803), 2014(179), 2021(2032), 2034(1223), 2081(143)

Table S23 Harmonic frequencies (cm^{-1}) and IR intensities (KM/Mole) of $Ru_3(CO)_{11}$ (**11-2**)

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
-23(0), 30(0), 36(0), 37(0), 41(0), 52(0), 68(0), 70(0), 74(0), 76(0), 88(0), 90(0), 91(0), 93(0), 96(0), 100(1), 108(0), 111(0), 114(0), 117(0), 139(0), 147(2), 148(0), 154(2), 190(0), 361(11), 391(0), 395(3), 396(0), 402(2), 405(1), 406(5), 418(11), 439(3), 442(1), 450(9), 455(1), 455(10), 459(6), 464(37), 465(14), 469(56), 476(14), 485(5), 492(25), 500(15), 513(6), 537(0), 539(0), 571(14), 574(39), 582(20), 585(16), 595(84), 603(58), 604(48), 624(245), 631(200), 2074(154), 2083(402), 2095(294), 2100(378), 2110(59), 2119(268), 2137(2787), 2137(121), 2147(2189), 2162(1804), 2219(69)	-22(0), 31(0), 35(0), 39(0), 42(0), 51(0), 66(0), 68(0), 72(0), 75(0), 86(0), 88(0), 89(0), 92(0), 93(0), 99(1), 107(0), 110(0), 113(0), 115(0), 138(0), 144(3), 148(0), 153(1), 183(0), 355(8), 376(0), 381(3), 382(0), 389(4), 390(1), 394(2), 405(11), 424(12), 428(0), 440(27), 440(1), 441(5), 445(7), 451(18), 454(43), 455(24), 464(11), 470(7), 477(17), 483(17), 504(4), 524(0), 525(0), 556(11), 558(35), 568(19), 576(17), 586(86), 593(4), 593(87), 608(188), 616(214), 2080(116), 2088(407), 2099(288), 2103(350), 2114(53), 2122(215), 2139(2768), 2140(78), 2150(2226), 2163(1742), 2219(62)	-21(0), 28(0), 32(0), 33(0), 38(0), 48(0), 64(0), 64(0), 69(0), 70(0), 80(0), 83(0), 86(0), 87(0), 90(0), 94(1), 98(1), 101(0), 104(0), 108(0), 127(0), 135(1), 136(0), 141(1), 174(0), 342(4), 366(2), 367(0), 373(0), 375(1), 384(0), 388(2), 399(1), 423(6), 433(1), 434(3), 435(28), 445(10), 448(1), 450(50), 452(11), 453(13), 459(10), 466(11), 477(7), 483(9), 499(1), 506(1), 510(0), 537(37), 539(11), 547(12), 558(28), 564(42), 573(69), 579(7), 590(148), 598(239), 1946(245), 1966(276), 1974(161), 1981(307), 1989(131), 1995(384), 2010(2255), 2012(52), 2023(1696), 2040(1415), 2088(60)	-20(0), 28(0), 30(0), 35(0), 39(0), 47(0), 63(0), 63(0), 68(0), 69(0), 79(0), 80(0), 83(0), 87(0), 87(1), 93(1), 98(1), 100(0), 104(0), 107(0), 127(0), 133(1), 136(0), 140(1), 169(0), 338(3), 352(3), 353(0), 360(0), 362(1), 371(0), 376(1), 387(1), 408(13), 420(33), 421(1), 423(1), 434(9), 436(2), 438(31), 440(13), 443(17), 449(7), 453(13), 464(5), 471(8), 491(1), 493(1), 497(0), 524(32), 525(8), 534(12), 552(13), 555(59), 563(51), 570(16), 576(117), 585(240), 1953(194), 1969(290), 1975(163), 1983(290), 1991(114), 1997(362), 2011(2251), 2014(38), 2026(1680), 2040(1367), 2087(51)

Table S24 Harmonic frequencies (cm^{-1}) and IR intensities (KM/Mole) of $Ru_3(CO)_{11}$ (**11-3**)

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
7(0), 40(0), 48(0), 56(0), 57(0), 57(0), 67(0), 68(0), 69(0), 77(0), 79(0), 81(1), 91(0), 94(0), 94(2), 94(0), 103(0), 104(0), 106(0), 113(0), 116(0), 148(6), 176(3), 236(0), 250(2), 355(1), 364(0), 380(6), 383(0), 393(21), 395(0), 406(0), 411(33), 421(31), 429(47), 439(3), 441(3), 442(1), 450(0), 453(0), 460(51), 478(52), 480(4), 490(22), 495(0), 513(3), 533(39), 540(0), 550(13), 553(52), 572(1), 576(0), 578(0), 580(85), 597(136), 605(19), 622(261), 638(19), 1937(213), 1955(794), 2097(0), 2104(1713), 2105(39), 2112(417), 2131(182), 2142(3259), 2162(978), 2165(1418), 2220(0)	-13(0), 39(0), 49(0), 55(0), 55(0), 55(0), 64(0), 67(0), 67(0), 74(0), 77(0), 80(1), 91(1), 91(0), 92(0), 93(0), 101(0), 101(0), 102(0), 112(0), 115(0), 142(5), 168(2), 230(0), 242(2), 348(1), 356(0), 373(3), 377(0), 382(0), 384(13), 393(0), 399(26), 409(40), 417(54), 428(1), 433(14), 434(0), 441(0), 443(4), 448(35), 464(43), 468(1), 477(24), 483(1), 507(10), 523(40), 526(0), 538(10), 549(42), 559(13), 562(0), 563(69), 566(1), 590(144), 595(5), 610(274), 626(18), 1950(222), 1968(752), 2103(0), 2108(1674), 2110(47), 2116(430), 2135(184), 2147(3161), 2167(873), 2168(1345), 2222(0)	6(0), 37(0), 44(0), 50(0), 54(0), 56(0), 65(0), 65(0), 67(0), 73(0), 75(0), 77(1), 83(0), 88(0), 88(1), 89(0), 96(0), 98(0), 102(0), 109(0), 111(0), 139(4), 164(3), 223(0), 238(1), 332(1), 345(0), 362(1), 374(1), 380(0), 384(4), 384(0), 395(0), 408(55), 414(24), 425(9), 428(2), 428(0), 434(0), 441(2), 448(20), 464(0), 465(54), 469(12), 486(0), 487(1), 507(20), 509(0), 518(11), 523(55), 544(3), 545(0), 546(1), 549(64), 569(89), 574(12), 590(195), 606(17), 1833(199), 1845(514), 1967(0), 1978(56), 1982(1205), 1988(298), 2004(148), 2011(2673), 2031(1069), 2040(1269), 2086(0)	-13(0), 37(0), 45(0), 49(0), 52(0), 54(0), 62(0), 64(0), 65(0), 70(0), 73(0), 75(1), 83(0), 85(0), 86(1), 88(0), 94(0), 97(0), 98(0), 108(0), 109(0), 134(3), 158(3), 218(0), 230(1), 328(1), 337(0), 355(1), 363(0), 371(0), 374(2), 374(0), 383(0), 399(52), 404(26), 414(17), 416(1), 422(1), 426(0), 432(0), 440(15), 453(0), 455(43), 462(15), 477(0), 480(0), 496(0), 499(21), 506(9), 521(49), 530(0), 531(0), 532(63), 541(0), 562(100), 565(3), 579(203), 597(18), 1846(202), 1857(490), 1972(0), 1982(49), 1985(1220), 1991(330), 2007(138), 2015(2611), 2036(942), 2042(1203), 2088(0)

Table S25 Harmonic frequencies (cm^{-1}) and IR intensities (KM/Mole) of $Ru_3(CO)_{11}$ (**11-4**)

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
-13(0), 12(0), 29(0), 47(0), 69(0), 72(0), 73(0), 75(0), 76(0), 81(0), 83(0), 89(0), 92(0), 94(0), 95(0), 101(0), 109(0), 123(0), 145(0), 160(0), 164(4), 180(1), 195(0), 211(0), 231(2), 317(0), 349(6), 370(13), 372(0), 381(3), 385(4), 394(6), 408(3), 425(13), 428(6), 432(11), 434(19), 443(0), 457(4), 461(7), 471(5), 472(0), 477(1), 489(1), 492(13), 492(2), 504(15), 507(3), 512(160), 539(8), 545(6), 556(177), 568(12), 573(45), 584(11), 586(208), 595(74), 611(306), 1831(485), 1892(248), 2103(20), 2118(169), 2127(129), 2130(128), 2134(666), 2142(1985), 2167(1933), 2171(2371), 2207(9)	-18(0), 8(0), 28(0), 46(0), 66(0), 69(0), 70(0), 73(0), 73(0), 79(0), 80(0), 86(1), 89(0), 90(0), 91(0), 98(0), 106(0), 123(0), 140(0), 155(0), 157(4), 170(0), 191(0), 204(0), 223(2), 306(1), 334(3), 355(17), 361(1), 368(4), 368(3), 376(6), 394(3), 409(11), 412(9), 416(16), 419(8), 429(0), 444(6), 446(5), 456(1), 461(1), 463(0), 470(2), 475(10), 479(1), 488(38), 492(130), 494(2), 522(12), 532(1), 536(157), 550(21), 556(17), 568(90), 570(103), 576(62), 594(302), 1856(480), 1913(259), 2107(27), 2121(131), 2131(146), 2133(132), 2137(652), 2146(1877), 2169(1868), 2173(2332), 2208(14)	-9(0), 6(0), 26(0), 43(0), 64(0), 68(0), 68(0), 70(0), 71(0), 76(0), 78(0), 84(0), 86(0), 89(0), 89(0), 95(0), 100(0), 118(0), 136(1), 147(0), 153(2), 166(2), 187(1), 194(0), 217(2), 310(0), 331(6), 350(6), 351(2), 359(0), 360(3), 377(4), 384(1), 404(3), 406(15), 415(4), 419(15), 423(1), 433(0), 448(6), 454(0), 456(3), 463(4), 464(2), 476(0), 477(2), 481(12), 487(119), 491(3), 511(5), 520(8), 525(174), 537(14), 539(18), 552(24), 554(164), 563(105), 576(209), 1729(305), 1794(211), 1975(8), 1990(103), 1998(189), 2000(178), 2004(627), 2011(1590), 2038(1594), 2042(1900), 2073(14)	-15(0), -11(0), 23(0), 42(0), 61(0), 65(0), 66(0), 67(0), 69(0), 74(0), 75(0), 81(0), 83(0), 85(0), 85(0), 93(0), 98(0), 119(0), 130(1), 142(0), 146(3), 157(1), 183(1), 187(0), 209(2), 299(0), 318(4), 335(9), 339(2), 345(1), 346(0), 360(4), 374(1), 388(3), 390(18), 399(1), 405(13), 409(0), 419(1), 434(6), 437(0), 443(9), 449(3), 452(10), 465(0), 466(0), 467(15), 471(98), 479(2), 498(10), 507(4), 508(153), 519(16), 524(6), 537(40), 539(127), 545(92), 560(209), 1751(293), 1817(225), 1977(11), 1991(65), 2000(232), 2002(184), 2006(617), 2013(1465), 2039(1553), 2042(1875), 2072(21)

Table S26 Harmonic frequencies (cm^{-1}) and IR intensities (KM/Mole) of $Ru_3(CO)_{10}$ (**10-1**)

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
8(0), 27(0), 44(0), 49(0), 63(0), 71(1), 76(0), 80(0), 81(0), 82(0), 85(0), 91(1), 95(0), 95(0), 98(0), 106(0), 142(0), 146(2), 156(0), 167(1), 184(0), 197(3), 208(0), 312(1), 327(33), 346(14), 359(10), 396(3), 399(6), 413(16), 424(4), 430(6), 436(3), 439(1), 447(4), 455(13), 464(5), 470(9), 478(31), 484(10), 488(5), 502(43), 523(9), 527(1), 538(65), 556(54), 567(103), 571(83), 577(17), 581(83), 591(208), 614(10), 625(113), 1923(384), 1979(299), 2014(1301), 2047(196), 2104(340), 2118(555), 2133(580), 2147(2595), 2158(2379), 2194(46)	17(1), 31(0), 41(0), 48(0), 57(0), 65(0), 69(1), 76(0), 78(0), 79(0), 84(0), 85(0), 89(0), 93(0), 94(0), 95(0), 115(1), 142(1), 148(1), 156(1), 194(1), 199(1), 218(0), 306(4), 329(5), 343(28), 363(15), 380(8), 393(9), 407(4), 416(2), 418(3), 427(4), 436(3), 437(4), 441(11), 446(12), 453(7), 461(4), 470(41), 487(19), 499(4), 504(11), 514(4), 531(39), 541(56), 548(94), 563(150), 568(60), 579(38), 579(127), 603(65), 633(149), 1926(412), 1970(397), 2045(1004), 2088(213), 2103(465), 2122(506), 2137(431), 2149(2564), 2160(2149), 2196(78)	18(0), 35(0), 43(0), 48(0), 61(0), 70(0), 75(0), 77(0), 80(0), 81(0), 84(0), 86(0), 91(0), 94(0), 97(0), 112(0), 132(0), 146(0), 166(0), 173(2), 180(0), 197(2), 204(0), 290(1), 309(22), 325(10), 338(10), 358(3), 373(7), 384(18), 389(2), 395(8), 410(2), 414(1), 432(5), 440(4), 451(1), 465(7), 468(17), 477(13), 482(19), 489(48), 493(1), 499(53), 505(4), 522(64), 527(34), 544(15), 547(7), 560(24), 565(199), 575(78), 580(2), 1829(284), 1868(146), 1878(1026), 1905(233), 1982(213), 1994(397), 1999(645), 2021(2164), 2030(1962), 2061(8)	21(0), 31(0), 40(0), 45(0), 60(0), 67(0), 71(0), 74(0), 77(0), 78(0), 80(0), 84(0), 88(0), 90(0), 94(0), 108(0), 127(0), 136(0), 157(0), 167(2), 170(0), 191(2), 198(0), 274(2), 303(20), 314(11), 321(3), 353(8), 361(7), 369(15), 380(5), 389(2), 394(4), 403(0), 421(6), 430(3), 441(1), 456(5), 460(13), 465(13), 473(6), 482(31), 485(12), 488(52), 498(8), 511(64), 519(34), 531(11), 535(21), 548(28), 550(176), 564(6), 567(74), 1834(316), 1870(153), 1888(985), 1918(230), 1984(204), 1997(362), 2003(592), 2022(2099), 2032(1944), 2062(10)

Table S27 Harmonic frequencies (cm^{-1}) and IR intensities (KM/Mole) of $Ru_3(CO)_{10}$ (**10-2**)

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
-39(1), 34(0), 43(0), 44(0), 59(0), 66(0), 76(1), 80(0), 81(0), 84(0), 85(0), 90(0), 93(0), 100(0), 101(0), 104(0), 131(1), 152(0), 161(0), 163(0), 184(0), 192(2), 214(0), 310(0), 310(20), 335(11), 344(0), 374(27), 376(12), 407(1), 411(6), 412(5), 425(4), 429(11), 454(0), 459(0), 460(2), 476(7), 484(21), 488(11), 506(17), 508(59), 516(44), 530(21), 542(110), 554(1), 559(44), 572(51), 576(1), 588(22), 595(281), 604(75), 613(29), 1967(495), 1972(4), 1993(1428), 2029(363), 2105(216), 2121(333), 2131(688), 2143(2858), 2158(2560), 2194(15)	-58(2), 30(0), 39(0), 42(0), 51(0), 68(0), 73(0), 77(0), 78(0), 81(0), 87(0), 91(0), 93(0), 95(0), 104(0), 108(0), 122(0), 137(1), 153(1), 161(0), 177(1), 185(3), 211(0), 277(11), 304(0), 326(10), 333(2), 368(31), 368(14), 391(5), 401(6), 414(7), 417(3), 422(12), 445(2), 447(0), 454(0), 466(28), 469(1), 476(5), 495(12), 496(41), 510(21), 518(47), 526(70), 542(9), 544(63), 565(64), 568(31), 574(15), 585(240), 593(5), 600(95), 1957(701), 1959(0), 2003(1276), 2042(394), 2107(171), 2125(305), 2138(716), 2147(2642), 2163(2455), 2197(33)	-16(1), 36(0), 41(0), 44(0), 63(0), 63(0), 73(1), 77(0), 80(0), 80(0), 83(0), 86(0), 89(0), 94(0), 98(0), 99(0), 135(1), 145(0), 162(0), 171(2), 181(0), 195(1), 204(0), 293(0), 315(18), 321(6), 330(4), 354(20), 359(8), 381(0), 390(9), 391(7), 407(2), 409(6), 437(3), 442(0), 446(2), 464(6), 475(21), 480(12), 490(38), 490(51), 491(0), 501(10), 513(93), 519(4), 530(27), 538(33), 544(3), 561(15), 565(191), 571(60), 581(41), 1851(441), 1858(5), 1877(1001), 1907(239), 1981(190), 1994(359), 1998(664), 2018(2259), 2030(1996), 2060(2)	-25(1), 35(0), 39(0), 40(0), 59(0), 61(0), 70(0), 74(0), 77(0), 78(0), 81(0), 84(0), 87(0), 91(0), 95(0), 95(0), 131(0), 135(0), 157(0), 165(2), 176(0), 190(1), 197(0), 278(0), 286(15), 312(8), 316(6), 345(18), 354(8), 372(3), 378(8), 378(3), 395(4), 396(5), 429(3), 432(1), 434(2), 455(6), 467(21), 471(10), 481(29), 482(44), 483(7), 489(6), 500(76), 510(3), 516(32), 530(30), 535(1), 550(19), 553(191), 561(60), 564(20), 1853(502), 1860(4), 1886(932), 1916(256), 1983(186), 1997(321), 2002(619), 2020(2182), 2032(1959), 2061(3)

Table S28 Harmonic frequencies (cm^{-1}) and IR intensities (KM/Mole) of $Ru_3(CO)_{10}$ (**10-3**)

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
-16(0), 25(0), 38(0), 58(0), 64(0), 71(0), 74(0), 76(0), 82(0), 87(0), 91(0), 91(0), 95(0), 100(0), 102(0), 113(0), 116(0), 142(1), 156(0), 169(0), 203(1), 206(1), 221(0), 287(1), 323(2), 378(1), 385(0), 391(5), 399(0), 407(6), 412(0), 428(62), 439(5), 440(20), 447(2), 448(31), 457(13), 466(0), 482(12), 483(18), 496(6), 496(5), 507(17), 525(11), 535(8), 545(0), 548(95), 556(27), 575(40), 575(0), 592(68), 599(186), 620(206), 1840(473), 1947(388), 2096(116), 2109(47), 2118(330), 2125(263), 2134(1192), 2146(2785), 2167(2239), 2200(81)	-21(0), 26(0), 33(0), 57(0), 62(0), 67(0), 72(0), 74(0), 80(0), 85(0), 88(0), 88(0), 95(0), 98(0), 100(0), 111(0), 115(0), 147(1), 151(0), 169(0), 194(1), 199(1), 213(0), 263(1), 319(2), 365(2), 371(0), 378(6), 387(1), 392(4), 396(0), 410(65), 423(6), 425(11), 426(26), 436(0), 447(12), 450(0), 468(16), 476(9), 482(8), 483(2), 498(9), 513(12), 518(8), 533(94), 533(0), 545(38), 559(42), 562(0), 578(37), 584(161), 606(191), 1869(492), 1945(373), 2101(124), 2115(37), 2123(309), 2130(239), 2138(1148), 2150(2668), 2171(2165), 2201(80)	-12(0), 25(0), 35(0), 54(0), 59(0), 67(0), 69(0), 70(0), 79(0), 82(0), 86(0), 87(0), 89(0), 94(0), 96(0), 104(0), 110(0), 127(1), 145(0), 153(0), 194(0), 197(0), 205(0), 276(2), 301(2), 355(1), 360(0), 371(0), 371(3), 388(2), 391(2), 405(45), 412(7), 415(11), 427(16), 428(3), 447(9), 454(2), 468(15), 471(2), 478(0), 479(3), 493(5), 504(22), 512(8), 520(60), 527(4), 527(22), 541(0), 545(25), 560(102), 570(145), 580(123), 1730(324), 1851(304), 1968(96), 1980(41), 1990(328), 1996(280), 2004(981), 2016(2298), 2040(1755), 2067(93)	-13(0), 26(0), 31(0), 52(0), 57(0), 63(0), 66(0), 68(0), 77(0), 80(0), 83(0), 84(0), 88(0), 91(0), 94(0), 103(0), 109(0), 133(1), 141(0), 151(0), 188(1), 189(0), 199(0), 255(1), 296(1), 343(1), 348(0), 359(3), 359(0), 375(2), 377(1), 385(44), 396(9), 401(8), 410(11), 418(1), 438(9), 440(2), 455(11), 465(3), 467(0), 468(4), 482(4), 492(22), 499(9), 509(54), 516(26), 518(7), 528(0), 532(38), 547(67), 557(123), 568(117), 1756(334), 1850(289), 1971(91), 1983(34), 1994(337), 1999(263), 2006(935), 2019(2204), 2042(1716), 2067(89)

Table S29 Harmonic frequencies (cm^{-1}) and IR intensities (KM/Mole) of $Ru_3(CO)_{10}$ (**10-4**)

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
11(1), 24(0), 35(0), 51(0), 52(0), 58(1), 67(0), 70(0), 71(1), 78(0), 81(0), 82(0), 86(0), 90(0), 99(0), 99(0), 102(0), 149(1), 154(0), 173(2), 203(1), 208(5), 211(10), 359(4), 359(11), 367(29), 375(5), 381(3), 393(2), 399(0), 405(1), 410(2), 432(92), 438(0), 441(59), 442(120), 451(80), 455(44), 463(1), 488(69), 494(0), 506(34), 506(1), 521(20), 545(72), 554(3), 555(33), 573(103), 596(1), 606(139), 632(15), 656(61), 659(21), 1960(1238), 1961(1283), 2007(8), 2091(24), 2093(742), 2130(1842), 2138(957), 2140(1976), 2150(874), 2199(140)	15(0), 30(0), 39(0), 50(0), 52(0), 57(1), 65(0), 68(1), 69(0), 78(0), 80(0), 81(0), 83(0), 89(0), 96(0), 98(0), 99(0), 139(1), 145(0), 173(2), 189(1), 200(5), 203(8), 337(11), 343(7), 347(22), 362(5), 375(9), 376(2), 388(2), 400(2), 401(3), 420(87), 425(89), 427(76), 431(40), 445(43), 448(22), 456(1), 470(31), 480(0), 489(2), 495(32), 511(23), 534(61), 551(2), 552(28), 562(61), 585(1), 594(148), 621(17), 637(57), 640(18), 1972(1186), 1973(1243), 2017(11), 2095(31), 2096(637), 2131(1815), 2139(905), 2143(1946), 2153(867), 2199(120)	-16(1), 19(0), 32(0), 41(0), 48(0), 49(0), 62(0), 67(0), 69(1), 74(0), 77(0), 79(0), 82(0), 86(0), 93(0), 94(0), 96(0), 141(1), 146(0), 173(3), 193(1), 198(2), 204(4), 314(0), 343(2), 348(37), 351(11), 364(1), 370(3), 376(1), 383(0), 387(0), 403(9), 406(5), 419(111), 424(99), 430(37), 434(0), 450(7), 463(0), 466(79), 486(1), 503(27), 506(0), 510(58), 539(63), 542(16), 544(68), 571(1), 577(76), 605(15), 630(47), 633(16), 1846(888), 1855(968), 1884(26), 1966(26), 1969(653), 2005(1550), 2012(725), 2018(1576), 2027(813), 2067(147)	-14(1), 25(0), 34(0), 37(0), 44(0), 50(0), 61(0), 65(1), 66(0), 73(0), 75(0), 76(0), 79(0), 84(0), 90(0), 92(0), 93(0), 131(1), 139(0), 169(2), 179(1), 190(2), 197(4), 295(1), 328(4), 329(36), 331(11), 353(3), 355(1), 368(5), 378(1), 380(1), 398(19), 400(1), 408(96), 409(91), 417(35), 427(1), 444(4), 451(0), 457(47), 474(2), 488(20), 490(1), 500(55), 532(87), 539(1), 540(16), 561(0), 565(85), 594(15), 613(40), 616(14), 1857(852), 1866(948), 1894(30), 1969(44), 1970(578), 2003(1483), 2011(708), 2020(1583), 2028(791), 2067(124)

Table S30 Harmonic frequencies (cm^{-1}) and IR intensities (KM/Mole) of $Ru_3(CO)_{10}$ (**10-5**)

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
12(0), 22(0), 22(0), 57(0), 68(0), 70(0), 70(0), 83(1), 83(1), 86(0), 94(0), 95(1), 95(1), 102(1), 102(1), 136(0), 136(0), 140(0), 167(1), 167(1), 210(0), 210(0), 214(0), 379(0), 379(0), 380(0), 396(0), 398(0), 398(0), 408(0), 436(1), 438(16), 438(16), 446(19), 446(19), 462(0), 484(28), 490(0), 490(0), 498(118), 504(4), 504(4), 516(5), 516(5), 529(19), 547(0), 547(0), 561(0), 574(142), 574(142), 589(0), 596(173), 596(173), 1868(384), 2086(0), 2099(3), 2099(3), 2123(266), 2123(266), 2128(2262), 2160(2378), 2160(2377), 2199(2)	9(0), 20(0), 20(0), 56(0), 66(0), 68(0), 68(0), 81(0), 81(0), 84(0), 92(0), 94(1), 94(1), 99(1), 99(1), 137(0), 137(0), 142(0), 159(1), 159(1), 201(0), 201(0), 204(0), 362(0), 362(0), 365(0), 383(0), 385(1), 385(1), 394(0), 419(1), 423(8), 423(8), 428(27), 428(27), 443(0), 471(59), 481(2), 481(2), 484(80), 490(4), 490(4), 505(7), 505(7), 520(11), 533(2), 533(2), 547(0), 554(120), 554(120), 569(0), 578(159), 578(159), 1898(391), 2090(0), 2103(0), 2103(0), 2126(269), 2126(269), 2132(2177), 2163(2315), 2163(2315), 2199(1)	10(0), 22(0), 22(0), 52(0), 65(0), 67(0), 67(0), 78(0), 78(0), 81(0), 89(0), 90(0), 90(0), 96(1), 96(1), 127(0), 127(0), 131(0), 154(1), 154(1), 196(0), 202(0), 202(0), 361(0), 361(0), 366(0), 375(0), 379(0), 379(0), 385(0), 413(0), 418(26), 418(26), 427(1), 427(1), 448(0), 462(52), 477(7), 477(7), 483(1), 483(1), 488(61), 504(9), 504(9), 509(9), 519(0), 519(0), 537(0), 542(94), 542(94), 554(0), 565(151), 565(151), 1741(259), 1960(0), 1973(6), 1973(6), 1995(224), 1995(224), 1999(1908), 2034(1865), 2034(1865), 2066(2)	7(0), 20(0), 20(0), 49(0), 62(0), 64(0), 64(0), 76(0), 76(0), 79(0), 86(0), 90(1), 90(1), 93(1), 93(1), 128(0), 128(0), 132(0), 147(1), 147(1), 184(0), 194(0), 194(0), 346(0), 346(0), 350(0), 363(0), 365(0), 365(0), 372(0), 396(0), 402(25), 402(25), 411(2), 411(2), 432(0), 448(65), 467(13), 467(13), 471(1), 471(1), 477(41), 494(12), 494(12), 503(5), 506(0), 506(0), 523(73), 523(74), 525(0), 536(0), 549(137), 549(137), 1769(265), 1962(0), 1975(2), 1975(2), 1997(216), 1997(216), 2001(1844), 2035(1827), 2035(1827), 2065(1)

Table S31 Harmonic frequencies (cm^{-1}) and IR intensities (KM/Mole) of $Ru_3(CO)_9$ (**9-1**)

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
33(0), 39(0), 45(0), 48(0), 53(0), 61(0), 71(0), 76(0), 77(0), 81(0), 91(0), 93(1), 94(0), 100(0), 102(0), 108(0), 114(0), 148(1), 158(2), 198(0), 204(2), 339(12), 364(9), 381(7), 394(12), 400(17), 419(16), 425(27), 432(29), 445(8), 451(4), 452(3), 466(18), 473(8), 481(10), 489(47), 495(4), 515(12), 518(1), 550(4), 565(34), 571(13), 583(130), 596(61), 599(38), 606(8), 615(10), 633(109), 1950(499), 2066(285), 2083(42), 2096(1145), 2104(608), 2122(2501), 2135(1997), 2158(606), 2202(93)	34(0), 37(0), 46(0), 47(0), 52(0), 59(0), 70(0), 74(0), 76(0), 80(0), 88(0), 91(0), 92(0), 98(0), 100(0), 106(0), 114(1), 142(1), 152(1), 193(1), 201(1), 329(8), 358(8), 371(8), 384(12), 390(15), 408(8), 415(34), 421(26), 435(7), 445(5), 446(2), 458(18), 463(4), 473(10), 480(35), 486(4), 501(16), 510(1), 540(2), 554(29), 564(11), 576(133), 584(60), 588(22), 596(13), 606(17), 620(112), 1956(482), 2072(291), 2088(36), 2101(1184), 2110(579), 2127(2401), 2139(1894), 2162(577), 2205(97)	30(0), 33(0), 42(0), 45(0), 50(0), 59(0), 65(0), 67(0), 74(0), 75(0), 85(0), 86(1), 87(0), 93(0), 97(0), 100(0), 126(2), 143(1), 156(1), 194(1), 195(0), 303(2), 347(3), 366(9), 372(12), 385(7), 393(3), 406(24), 417(27), 429(10), 436(14), 443(2), 446(3), 456(2), 460(17), 470(41), 478(4), 485(11), 504(1), 520(2), 535(37), 548(101), 550(18), 561(19), 563(36), 571(19), 581(16), 593(67), 1846(345), 1914(334), 1966(44), 1976(495), 1979(853), 1997(1695), 2009(2032), 2029(457), 2071(131)	31(0), 32(0), 42(0), 43(0), 50(0), 57(0), 65(0), 66(0), 73(0), 75(0), 83(0), 84(0), 86(0), 91(0), 95(0), 99(0), 124(2), 138(1), 153(1), 185(1), 193(1), 297(2), 342(2), 356(9), 365(11), 377(6), 384(3), 398(22), 408(27), 420(10), 431(14), 438(0), 440(4), 449(2), 452(15), 463(28), 471(10), 477(14), 498(2), 513(1), 526(26), 542(126), 544(9), 551(18), 554(27), 561(17), 574(26), 584(66), 1854(332), 1922(331), 1970(42), 1981(618), 1982(736), 2000(1649), 2013(1919), 2033(436), 2073(129)

Table S32 Harmonic frequencies (cm^{-1}) and IR intensities (KM/Mole) of $Ru_3(CO)_9$ (**9-2**)

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
21(0), 32(0), 45(0), 52(0), 72(0), 73(0), 78(0), 82(0), 85(0), 88(1), 91(0), 94(0), 102(0), 104(1), 128(0), 150(0), 171(0), 213(1), 222(1), 224(0), 226(1), 245(0), 357(66), 374(1), 382(0), 390(0), 406(11), 408(0), 433(20), 433(0), 439(4), 444(10), 452(0), 455(32), 477(8), 482(34), 491(6), 504(0), 521(3), 525(36), 546(115), 554(14), 556(13), 578(75), 585(128), 631(1), 641(172), 668(87), 1906(968), 1913(8),	21(0), 31(0), 45(0), 51(0), 70(0), 72(0), 76(0), 83(0), 83(0), 86(0), 90(0), 91(0), 103(0), 104(1), 128(0), 144(0), 168(0), 207(1), 214(1), 218(1), 221(1), 239(0), 340(65), 363(1), 373(0), 378(0), 387(8), 404(0), 415(15), 424(0), 429(3), 433(2), 442(0), 445(34), 472(35), 472(7), 483(6), 495(0), 507(12), 517(32), 534(84), 542(11), 544(14), 565(70), 574(113), 616(9), 630(138), 659(104), 1914(969), 1921(9), 1975(829),	8(0), 32(0), 45(0), 50(0), 69(0), 70(0), 73(0), 76(0), 78(0), 84(0), 88(0), 89(0), 94(0), 96(1), 121(0), 144(1), 171(0), 204(0), 209(1), 214(1), 222(0), 235(0), 347(29), 353(0), 362(3), 366(0), 385(0), 392(11), 409(1), 418(13), 419(2), 429(0), 429(8), 435(14), 460(32), 463(6), 480(0), 481(2), 487(3), 509(18), 514(81), 533(11), 536(38), 544(60), 557(105), 599(13), 609(130), 633(46), 1802(709), 1810(9), 1843(672),	11(0), 31(0), 44(0), 50(0), 67(0), 68(0), 71(0), 78(0), 78(0), 82(0), 86(0), 87(0), 94(0), 97(1), 120(0), 138(0), 170(0), 199(0), 201(1), 204(1), 215(0), 229(0), 334(31), 346(0), 353(4), 356(0), 374(8), 382(0), 401(0), 405(12), 411(2), 418(6), 421(0), 426(12), 450(31), 459(5), 472(3), 473(3), 477(4), 501(15), 505(64), 522(11), 529(36), 534(55), 548(90), 589(1), 599(119), 625(59), 1809(704), 1817(9), 1857(661),

1962(860), 1994(399), 2117(275), 2126(1335), 2129(1540), 2156(2205), 2186(228)	2006(435), 2121(278), 2130(1274), 2134(1458), 2160(2143), 2189(226)	1866(264), 1988(127), 1993(1453), 1995(1230), 2029(1715), 2053(240)	1880(281), 1991(135), 1998(1182), 1998(1404), 2031(1665), 2055(234)

Table S33 Harmonic frequencies (cm^{-1}) and IR intensities (KM/Mole) of $Ru_3(CO)_9$ (**9-3**)

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
30(0), 30(0), 42(0), 47(0), 47(0), 51(1), 79(2), 79(2), 79(1), 88(0), 89(0), 89(0), 96(1), 96(1), 101(0), 125(0), 130(4), 130(4), 152(1), 152(1), 189(0), 326(8), 350(29), 350(29), 399(34), 399(34), 415(10), 415(10), 428(1), 432(0), 449(1), 456(14), 456(14), 471(18), 473(2), 473(2), 483(5), 483(5), 512(9), 542(16), 555(9), 555(9), 585(60), 585(60), 589(8), 603(4), 611(41), 611(41), 2024(152), 2024(152), 2038(1285), 2100(712), 2102(813), 2102(813), 2139(2307), 2139(2307), 2182(34)	29(0), 29(0), 42(0), 46(0), 46(0), 50(1), 74(2), 74(2), 78(1), 87(0), 87(0), 88(0), 94(0), 94(0), 99(0), 129(2), 129(2), 131(0), 152(2), 152(2), 179(0), 309(6), 332(27), 332(27), 395(18), 395(18), 407(19), 407(19), 422(0), 427(0), 446(0), 454(7), 454(7), 462(14), 463(3), 463(3), 476(6), 476(6), 504(10), 528(16), 548(14), 548(14), 574(49), 574(49), 579(9), 584(3), 598(50), 598(50), 2025(189), 2025(189), 2037(1264), 2107(643), 2108(817), 2108(816), 2146(2132), 2146(2132), 2185(48)	26(0), 26(0), 35(0), 46(0), 46(0), 47(1), 70(3), 70(3), 77(1), 85(0), 85(0), 85(0), 91(0), 91(0), 95(0), 120(0), 126(3), 126(3), 147(1), 147(1), 186(0), 297(5), 329(26), 329(26), 379(14), 379(14), 391(5), 391(5), 406(0), 412(1), 432(4), 432(4), 448(2), 452(4), 453(7), 453(7), 474(9), 474(9), 503(15), 516(11), 527(8), 527(8), 552(28), 552(28), 556(12), 565(0), 576(31), 576(31), 1905(120), 1905(120), 1916(985), 1972(770), 1972(770), 1973(649), 2011(1777), 2011(1777), 2048(72)	27(0), 27(0), 38(0), 45(0), 45(0), 47(1), 66(3), 66(3), 76(1), 83(0), 83(0), 87(0), 89(0), 89(0), 92(0), 125(2), 125(2), 128(0), 148(3), 148(3), 174(0), 285(4), 314(24), 314(24), 377(4), 377(4), 384(15), 384(15), 400(0), 410(0), 426(0), 426(0), 443(4), 448(0), 449(4), 449(4), 473(9), 473(9), 493(18), 510(7), 521(14), 521(14), 544(21), 544(21), 546(7), 550(5), 564(38), 564(38), 1904(137), 1904(137), 1915(951), 1978(734), 1978(734), 1980(593), 2017(1674), 2017(1674), 2050(81)

Table S34 Harmonic frequencies(cm^{-1}) and IR intensities (KM/Mole) of $Ru_3(CO)_9$ (**9-4**)

MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD	BP86/LANL2DZ
30(0), 33(0), 33(0), 49(0), 49(0), 56(0), 67(0), 67(0), 79(0), 79(0), 86(1), 95(0), 95(0), 99(0), 102(0), 102(0), 104(0), 114(0), 151(1), 151(1), 192(1), 354(2), 354(2), 359(29), 390(2), 390(2), 399(34), 417(2), 417(2), 438(28), 460(11), 460(11), 467(1), 467(1), 468(36), 492(1), 514(2), 515(4), 515(4), 552(30), 552(30), 565(16), 576(51), 583(11), 583(11), 610(37), 610(37),	30(0), 33(0), 33(0), 49(0), 49(0), 56(0), 66(0), 66(0), 78(0), 78(0), 84(1), 95(0), 95(0), 97(0), 99(0), 99(0), 103(0), 111(0), 145(1), 145(1), 182(1), 346(1), 346(1), 351(26), 382(2), 382(2), 390(32), 408(2), 408(2), 427(32), 453(11), 453(11), 460(1), 460(1), 460(29), 483(2), 506(1), 508(3), 508(3), 543(25), 543(25), 556(13), 568(52), 574(10), 574(10), 600(39), 600(39),	26(0), 26(0), 27(0), 46(0), 46(0), 52(0), 61(0), 61(0), 71(1), 71(1), 78(1), 88(0), 88(0), 91(0), 97(0), 97(0), 97(0), 103(0), 142(1), 142(1), 182(1), 340(1), 340(1), 344(9), 376(1), 376(1), 381(15), 406(1), 406(1), 424(42), 435(9), 435(9), 455(3), 455(3), 458(23), 470(1), 497(1), 500(2), 500(2), 528(30), 528(30), 537(35), 546(20), 551(3), 551(3), 574(32), 574(32), 578(2), 1949(32),	26(0), 26(0), 28(0), 46(0), 46(0), 52(0), 60(0), 60(0), 70(0), 70(0), 77(1), 88(0), 88(0), 90(0), 94(0), 94(0), 96(0), 101(0), 137(1), 137(1), 173(1), 333(1), 333(1), 337(7), 367(1), 367(1), 373(13), 399(1), 399(1), 416(44), 429(9), 429(9), 450(3), 450(3), 451(18), 464(1), 490(1), 495(2), 495(2), 521(28), 521(28), 529(38), 539(16), 543(1), 543(1), 566(35), 566(35), 569(1), 1955(31),

616(4), 2071(64), 2071(64), 2090(110), 2091(1290), 2091(1290), 2118(3248), 2151(848), 2151(848), 2207(65)	605(2), 2078(87), 2078(88), 2094(102), 2096(1229), 2096(1229), 2123(3199), 2156(805), 2156(805), 2209(60)	1949(32), 1972(29), 1972(968), 1972(968), 1989(2722), 2024(792), 2024(792), 2074(31)	1955(31), 1975(33), 1976(944), 1976(944), 1992(2674), 2028(747), 2028(747), 2076(29)

Table S1A. The total energies (*E*, in hartrees) and relative energies (Δ*E*, in kcal/mol) for $Ru_3(CO)_{12}$. The number of imaginary vibrational frequencies (Nimag) for each structure is also listed.

		12-1 (*D_3*)	**12-2** (*C_{2v}*)	**12-3** (*D_{3h}*)	**12-4** (*D_{3h}*)
MPW1PW91	–E total	1645.02489	1645.02199	1645.02166	1645.01750
/SDD	ΔE relative	0	1.8	2.0	4.6
	Nimag	0	1(15i)	1(14*i*)	0
BP86/SDD	–E total	1645.72438	1645.72391	1645.72080	1645.71902
	ΔE relative	0	0.3	2.2	3.4
	Nimag	0	0	1(14*i*)	0
MPW1PW91	–E total	1641.88324	1641.88053	1641.88018	1641.88112
/LANL2DZ	ΔE relative	0	1.7	1.9	1.3
	Nimag	0	1(33i)	1(16*i*)	0
BP86/LANL	–E total	1642.52654	1642.52621	1642.52322	1642.52496
2DZ	ΔE relative	0	0.2	2.1	1.0
	Nimag	0	0	1(15*i*)	0

Table S2A. Comparison of the experimental ν(CO) vibrational frequencies (cm^{-1}) with those predicted for the trinuclear $Ru_3(CO)_{12}$ isomers using all methods and both basis sets (predicted infrared intensities in parentheses are in km/mol).

	12-1 (D_3)	**12-2** (C_{2v})	**12-3** (D_{3h})	**12-4** (D_{3h})	Experimental
MPW1PW91/	2089(10)	1935(880)	2097(0)	1970(1330)	
SDD	2089(10)	1984(250)	2097(0)	1970(1330)	
	2104(4)	2109(75)	2099(0)	2012(0)	
	2110(262)	2112(4)	2114(20)	2113(0)	
	2110(262)	2121(624)	2114(20)	2113(0)	
	2120(81)	2126(0)	2117(485)	2118(975)	
	2120(81)	2127(167)	2117(485)	2118(975)	
	2129(3115)	2136(129)	2140(3053)	2130(0)	
	2132(0)	2141(2452)	2141(0)	2151(3186)	
	2158(2554)	2163(1969)	2163(2377)	2177(975)	
	2158(2554)	2164(2481)	2163(2376)	2177(975)	
	2218(0)	2217(58)	2225(0)	2228(0)	

MPW1PW91/	2092(15)	1948(884)	2099(0)	1983(1253)	
LANL2DZ	2092(15)	1994(256)	2099(0)	1983(1253)	
	2108(0)	2113(54)	2103(0)	2021(0)	
	2113(190)	2115(6)	2118(0)	2118(0)	
	2113(190)	2125(547)	2118(0)	2118(0)	
	2124(81)	2129(0)	2120(390)	2122(969)	
	2124(81)	2131(156)	2120(390)	2122(969)	
	2130(3069)	2139(109)	2141(3002)	2134(0)	
	2135(0)	2143(2386)	2144(0)	2155(3082)	
	2160(2526)	2165(1959)	2164(2400)	2179(941)	
	2160(2526)	2166(2438)	2164(2400)	2179(941)	
	2217(0)	2216(58)	2224(0)	2229(0)	
BP86/SDD	1968(7)	**1845(616)**	1975(0)	**1863(978)**	298 K:
	1968(7)	**1874(191)**	1975(0)	**1863(978)**	2011(9000),
	1981(9)	1985(78)	1978(0)	**1888(0)**	2017(3600),
	1989(396)	1986(2)	1991(30)	1986(0)	2031(14600),
	1989(396)	1996(690)	1991(30)	1986(0)	2061(24500)
	1997(34)	2000(0)	1995(558)	1995(686)	
	1997(34)	2000(146)	1995(558)	1995(686)	90 K:
	2005(2594)	2010(122)	2014(2529)	2006(0)	2008(12000),
	2008(0)	2014(2068)	2017(0)	2021(2694)	2017(6400),
	2036(1950)	2038(2088)	2042(1779)	2052(943)	2031(42000),
	2036(1950)	2040(1399)	2042(1779)	2052(943)	2063(48000)
	2088(0)	2084(69)	2094(0)	2096(0)	
BP86/LANL2	1970(10)	**1856(612)**	1976(0)	**1875(932)**	
DZ	1970(10)	**1883(192)**	1976(0)	**1875(932)**	
	1983(5)	1987(65)	1980(0)	**1898(0)**	
	1991(336)	1988(4)	1994(16)	1990(0)	
	1991(336)	1998(636)	1994(16)	1990(0)	
	1999(34)	2002(0)	1997(482)	1997(688)	
	1999(34)	2002(134)	1997(482)	1997(688)	
	2005(2550)	2012(106)	2014(2478)	2008(0)	
	2009(0)	2015(2016)	2018(0)	2023(2607)	
	2036(1930)	2038(2040)	2041(1796)	2053(907)	
	2036(1930)	2040(1384)	2041(1796)	2053(907)	
	2086(0)	2083(69)	2092(0)	2097(0)	

Table S3A The total energies (E, in hartrees) and relative energies (ΔE, in kcal/mol) for $Ru_3(CO)_{11}$. The number of imaginary vibrational frequencies (Nimag) for each structure is also listed.

		11-1 (C_1)	**11-2** (C_s)	**11-3** (C_{2v})	**11-4** (C_s)
MPW1PW91/SDD	–E total	1531.65561	1531.64986	1531.64564	1531.64518
	ΔE relative	0	3.6	6.3	6.5
	Nimag	0	1(23*i*)	0	1(13*i*)
BP86/SDD	–E total	1532.32473	1532.31773	1532.31771	1532.31971
	ΔE relative	0	4.4	4.4	3.2
	Nimag	0	1(21*i*)	0	1(8*i*)
MPW1PW91/LANL2DZ	–E total	1528.52338	1528.51801	1528.51823	1528.50596
	ΔE relative	0	3.4	3.2	10.9
	Nimag	0	1(22*i*)	1(13*i*)	1(18*i*)
BP86/LANL2DZ	–E total	1529.13564	1529.12921	1529.13199	1529.12438
	ΔE relative	0	4.0	2.3	7.1
	Nimag	0	1(20*i*)	1(13*i*)	2(15*i*,11*i*)

Table S4A The ν(CO) vibrational frequencies (cm^{-1}) predicted for the $Ru_3(CO)_{11}$ isomers.[a]

	BP86/SDD	BP86/LANL2DZ
11-1 (C_1)	**1861(402)**, 1936(398), 1974(207), 1983(259), 1986(83), 1993(126), 2008(1836), 2012(191), 2018(2088), 2033(1285), 2081(150)	**1870(407)**, 1941(389), 1978(207), 1985(273), 1989(73), 1996(113), 2009(1803), 2014(179), 2021(2032), 2034(1223), 2081(143),
11-2 (C_s)	1946(245), 1966(276), 1974(161), 1981(307), 1989(131), 1995(384), 2010(2255), 2012(52), 2023(1696), 2040(1415), 2088(60)	1953(194), 1969(290), 1975(163), 1983(290), 1991(114), 1997(362), 2011(2251), 2014(38), 2026(1680), 2040(1367), 2087(51)
11-3 (C_{2v})	**1833(199), 1845(514),** 1967(0), 1978(56), 1982(1205), 1988(298), 2004(148), 2011(2673), 2031(1069), 2040(1269), 2086(0)	**1846(202), 1857(490),** 1972(0), 1982(49), 1985(1220), 1991(330), 2007(138), 2015(2611), 2036(942), 2042(1203), 2088(0)
11-4 (C_s)	**1729(305), 1794(211),** 1975(8), 1990(103), 1998(189), 2000(178), 2004(627), 2011(1590), 2038(1594), 2042(1900), 2073(14)	**1751(293), 1817(225),** 1977(11), 1991(65), 2000(232), 2002(184), 2006(617), 2013(1465), 2039(1553), 2042(1875), 2072(21)
Expt **Error! Bookmark not defined.**	$Ru_3(CO)_{11}$ bridged form **1836(2300),** 1935(3000), 1975(3000), 2005(8300), 2023(9300), 2033(29000), 2039(4500), 2063(15000), 2107(2500) $Ru_3(CO)_{11}$ terminal form 1975(1300), 2011(9400), 2026(20000), 2033(16000), 2042(3400), 2054(23000), 2062(14000), 2110(2300), 2124(300) $Ru_3(CO)_{11}$ in 2-MeTHF **1824(5.8), 1831(5.8),** 1950(0.6), 1986(1.8), 2008(1.3), 2018(2.6), 2036(7.0), 2065(6.9), 2075(2.3), 2113(l.0)	

[a]For the theoretical ν(CO) frequencies the infrared intensities in parentheses are in km/mol; for the experimental ν(CO) frequencies the infrared intensities in parentheses are estimated extinction coefficients. Bridging ν(CO) frequencies are listed in **bold** type.

Table S5A The total energies (E, in hartrees) and relative energies (ΔE, in kcal/mol) for $Ru_3(CO)_{10}$. The number of imaginary vibrational frequencies (Nimag) for each structure is also listed.

		10-1 (C_1)	**10-2** (C_2)	**10-3** (C_s)	**10-4** (C_2)	**10-5** (C_{3v})
MPW1PW91/SDD	–E total	1418.32213	1418.32077	1418.31038	1418.30828	1418.30598
	ΔE relative	0	0.9	7.4	8.7	10.1
	Nimag	0	1(39*i*)	1(16*i*)	0	0
BP86/SDD	–E total	1418.96803	1418.96765	1418.95301	1418.94418	1418.94844
	ΔE relative	0	0.2	9.4	15.0	12.3
	Nimag	0	1(16*i*)	1(12*i*)	1(16*i*)	0
MPW1PW91/LANL2	–E total	1415.19425	1415.19200	1415.17798	1415.17778	1415.16798
DZ	ΔE relative	0	1.4	10.2	10.3	16.5
	Nimag	0	1(58*i*)	1(21*i*)	0	0
BP86/LANL2DZ	–E total	1415.78186	1415.78153	1415.76394	1415.75605	1415.75450
	ΔE relative	0	0.2	11.2	16.2	17.2
	Nimag	0	1(25*i*)	1(13*i*)	1(14*i*)	0

Table S6A The ν(CO) vibrational frequencies(cm^{-1}) predicted for the $Ru_3(CO)_{10}$ isomers (infrared intensities in parentheses are in km/mol, bridging ν(CO) frequencies are in bold).

	BP86/SDD	BP86/LANL2DZ
10-1 (C_1)	**1829(284)**,**1868(146)**,**1878(1026)**, **1905(233)**,1982(213),1994(397), 1999(645),2021(2164),2030(1962), 2061(8)	**1834(316)**,**1870(153)**,**1888(985)**, **1918(230)**,1984(204),1997(362), 2003(592),2022(2099),2032(1944), 2062(10)
10-2 (C_2)	**1851(441),1858(5),1877(1001), 1907(239)**,1981(190),1994(359), 1998(664),2018(2259),2030(1996), 2060(2)	**1853(502),1860(4),1886(932)**, **1916(256)**,1983(186),1997(321), 2002(619),2020(2182),2032(1959), 2061(3)
10-3 (C_s)	**1730(324),1851(304)**,1968(96), 1980(41),1990(328),1996(280), 2004(981),2016(2298),2040(1755), 2067(93)	**1756(334),1850(289)**,1971(91), 1983(34),1994(337),1999(263), 2006(935),2019(2204),2042(1716), 2067(89)
1**0-4** (C_2)	**1846(888),1855(968),1884(26)**, 1966(26),1969(653),2005(1550), 2012(725),2018(1576),2027(813), 2067(147)	**1857(852),1866(948),1894(30)**, 1969(44),1970(578),2003(1483), 2011(708),2020(1583),2028(791), 2067(124)
10-5 (C_{3v})	**1741(259)**,1960(0),1973(6), 1973(6),1995(224),1995(224), 1999(1908),2034(1865),2034(1865), 2066(2)	**1769(265)**,1962(0),1975(2), 1975(2),1997(216),1997(216), 2001(1844),2035(1827),2035(1827), 2065(1)

Table S7A The total energies (*E*, in hartrees) and relative energies (Δ*E*, in kcal/mol) for $Ru_3(CO)_9$. The number of imaginary vibrational frequencies (Nimag) for each structure is also listed.

		9-1 (C_1)	**9-2** (C_s)	**9-3** (C_3)	**9-4** (C_3)
MPW1PW91/SDD	–E total	1304.95739	1304.95278	1304.94077	1304.93410
	ΔE relative	0	2.9	10.4	14.6
	Nimag	0	0	0	0
BP86/SDD	–E total	1305.56086	1305.56638	1305.54729	1305.53778
	ΔE relative	0	–3.5	8.5	14.5
	Nimag	0	0	0	0
MPW1PW91/LANL2DZ	–E total	1301.84194	1301.83102	1301.82202	1301.82177
	ΔE relative	0	6.9	12.5	12.7
	Nimag	0	0	0	0
BP86/LANL2DZ	–E total	1302.38737	1302.38762	1302.37071	1302.36698
	ΔE relative	0	–0.2	10.5	12.8
	Nimag	0	0	0	0

Table S8A The ν(CO) vibrational frequencies (cm^{-1}) predicted for the $Ru_3(CO)_9$ isomers (infrared intensities in parentheses are in km/mol, bridging ν(CO) frequencies are in bold).

	BP86/SDD	BP86/LANL2DZ
9-1 (C_1)	**1846(345)**,**1914(334)**,1966(44), 1976(495),1979(853),1997(1695), 2009(2032),2029(457),2071(131)	**1854(332)**,**1922(331)**,1970(42), 1981(618),1982(736),2000(1649), 2013(1919),2033(436),2073(129)
9-2 (C_s)	**1802(709),1810(9),1843(672), 1866(264),**1988(127),1993(1453), 1995(1230),2029(1715),2053(240)	**1809(704),1817(9),1857(661), 1880(281),**1991(135),1998(1182), 1998(1404),2031(1665),2055(234)
9-3 (C_3)	**1905(120),1905(120),1916(985)**, 1972(770),1972(770),1973(649), 2011(1777),2011(1777),2048(72)	**1904(137),1904(137),1915(951)**, 1978(734),1978(734),1980(593), 2017(1674),2017(1674),2050(81)
9-4 (C_3)	1949(32),1949(32),1972(29), 1972(968),1972(968),1989(2722), 2024(792),2024(792),2074(31)	1955(31),1955(31),1975(33), 1976(944),1976(944),1992(2674), 2028(747),2028(747),2076(29)

Complete Gaussian 03 reference

(Reference 29)

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