Supporting Information

Electronic Structures and Binding Properties of Chalcogenolate-Bridged Molecular Wheels of Ruthenium and Osmium

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Selection of Method for Geometry Optimization

In order to choose the most appropriate method for the calculations of the molecular wheel complexes, geometry optimization of the simple model compound, $[Ru(SMe)_2(CO)_2]_6$, was undertaken. We used density functionals in combination with two types of basis sets. One is split valence def2-SVP[1] basis set (with a 31111/411/41/1 contraction and the Stuttgart-Dresden-Dunning (SDD) relativistic effective core potential (RECP)[2] for Ru) (denoted as BS1) and the other is LANL2DZ RECP basis set[3] for Ru and 6-311G(d) for S, C, O and H (denoted as BS2). The test functionals included local spin density approximation (LSDA) functionals, generalized gradient approximations (GGAs), hybrid GGAs, meta GGAs, and hybrid meta GGAs. The LSDA that we used was SWVN5[4] The four GGA methods we used for the testing calculations were BP86,[5, 6] PBE,[7, 8] OLYP[9, 10] and HCTH.[11] The meta DFT methods that we have tested were TPSS (TPSS exchange with TPSS correlation, also called TPSSTPSS),[12] and VSXC.[13] The hybrid GGA methods used for the calculations were O3LYP[9, 10, 14], B3LYP,[6, 10, 15] PBE0,[7, 16] BH&HLYP[6, 10, 15] and MPW1K.[17, 18] And four hybrid meta GGAs, namely TPSSh,[12] BB1K,[6, 19, 20] MPW1B95, [17, 19, 20] and PBE1KCIS.[7, 21] have been chosen. The local minima of all of the optimized structures were verified by evaluation of the harmonic vibrational frequencies. The local minima of all optimized structures were verified by evaluation of the harmonic vibrational frequencies. Among all combinations, PBE/BS1, PBE0/BS1 and PBE0/BS2 gave the best results when compared with experimental data (Table S1-S2, Fig. S1).

Table S1. Selected bond length (Å) and bond angle (º) of $[Ru(SMe)_2(CO)_2]_6$ calculated by different density functional methods; the experimental average values determined by X-ray crystallography are included for comparison.

Method	Ru-Ru	Ru-S1	Ru-S2	Ru-C1	S1-S2	<Ru-S1-Ru	<Ru-S2-Ru	<S-Ru-S(trans)
SVWN5/BS1	3.600	2.443	2.292	1.844	3.192	97.6	94.9	163.7
SVWN5/BS2	3.619	2.451	2.411	1.864	3.212	97.3	95.2	164.0
BP86/BS1	3.739	2.505	2.450	1.870	3.223	99.4	96.5	165.7
BP86/BS2	3.759	2.516	2.474	1.890	3.254	98.9	96.7	164.2
PBE/BS1	3.718	2.498	2.442	1.866	3.221	99.1	96.2	163.7
PBE/BS2	3.742	2.509	2.466	1.886	3.251	98.7	96.4	164.3
OLYP/BS1	3.787	2.514	2.451	1.857	3.188	101.2	97.7	163.7
OLYP/BS2	3.814	2.529	2.479	1.876	3.225	100.6	98.0	164.5
HCTH/BS1	3.785	2.520	2.454	1.850	3.206	100.9	97.3	164.3
HCTH/BS2	3.813	2.536	2.482	1.870	3.244	100.4	97.5	165.0
TPSS/BS1	3.713	2.494	2.447	1.879	3.226	98.7	96.2	163.7
TPSS/BS2	3.733	2.504	2.469	1.900	3.256	98.2	96.4	164.5
O3LYP/BS1	3.756	2.498	2.442	1.858	3.186	100.6	97.5	164.1
O3LYP/BS2	3.780	2.511	2.468	1.879	3.220	100.0	97.7	165.0
B3LYP/BS1	3.756	2.510	2.466	1.881	3.241	99.2	96.9	164.9
B3LYP/BS2	3.776	2.522	2.491	1.904	3.276	98.5	96.9	165.6
BH&HLP/BS1	3.716	2.482	2.453	1.895	3.227	98.5	97.0	166.3
BH&HLP/BS2	3.730	2.490	2.476	1.922	3.262	97.7	97.0	167.0
PBE0/BS1	3.675	2.466	2.422	1.865	3.195	98.7	96.3	164.5
PBE0/BS2	3.692	2.474	2.443	1.887	3.223	98.2	96.5	165.2
Exp	3.703	2.473	2.418	1.857	3.171	99.9	97.0	164.2

Table S2. PBE0 calculated Structural Parameters of the RuS_2 Units for the Ruthium-Thiolate Hexamer, Octamer and dodecamer (bond length in Å, bond angle in degree)

	$[Ru(\mu\text{-}SMe)_2(CO)_2]_6$		$[Ru(\mu\text{-}SMe)_2(CO)_2]_8$		$[Ru(\mu\text{-}SMe)_2(CO)_2]_{10}$		$[Ru(\mu\text{-}SMe)_2(CO)_2]_{12}$	
	LanL2dz/6-311g(d)	SVP	LanL2dz/6-311g(d)	SVP	LanL2dz/6-311g(d)	SVP	LanL2dz/6-311g(d)	SVP
Ru-Ru	3.692(3.703)*	3.675	3.660(3.666) *	3.648	3.665	3.655	3.667	3.656
Ru-S1	2.474(2.473)	2.466	2.490(2.492)	2.482	2.500	2.494	2.510	2.505
Ru-S2	2.443(2.418)	2.422	2.435(2.412)	2.414	2.436	2.415	2.439	2.417
Ru-C1	1.887(1.870)	1.865	1.886(1.899)	1.864	1.885	1.862	1.883	1.860
S1-S2	3.223(3.171)	3.195	3.184(3.120)	3.153	3.123	3.089	3.080	3.048
<Ru-S1-Ru	96.5(97.0)	96.3	94.6(94.7)	94.6	94.3	94.3	93.8	93.7
<Ru-S2-Ru	98.2(99.9)	98.7	97.5(98.8)	98.1	97.6	98.3	97.5	98.3
<S-Ru-S(trans)	165.2(164.2)	164.5	167.2(163.8)	166.4	167.6	166.7	167.5	166.4

***X-ray Structural average value in parentheses**

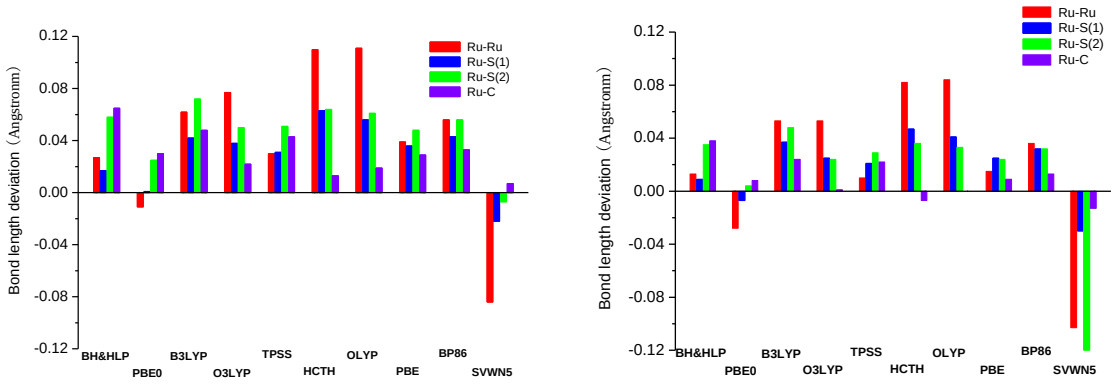

Fig. S1. Variation in bond length s(Å) relative to the experimental average values, using various DFT functionals at LanL2DZ/6-311g(d) (left) and def2-SVP (right) basis set.

Calculations of Bindings of Small Molecules and Alkali Metal Ions

For calculating the energies of bindings of alkali metal ions with the molecular wheels, the DFT functionals were evaluated at PBE0/BS1 levels of theory with basis set superposition error (BSSE) by means of the counterpoise (CP) procedure[22] implemented in Gaussian 03 program[23]. For the bindings of small gas molecules, DFT calculations were performed using the Amsterdam Density Functional ADF2012 program[24,25] developed by Baerends, Ziegler, and co-workers. The unrestricted Becke Perdew exchange-correlation potential was employed to optimize geometry without symmetry constraint. Relativistic corrections were introduced by scalar-relativistic zero-order regular approximation (ZORA)[26]. A full electronic triple-ζ basis set plus one polarization function were used for all atoms. To evaluate covalent or non-covalent attachment, Grimme's dispersion correction DFT-D3 was implemented[27].

Cartesian Coordinate of Optimized Geometries by PBE0/BS1

$[Fe(SMe)_2(CO)_2]_6$

E =-7354.913194 a.u.

Fe,1.7474292917,3.0266363191,0.
Fe,-1.7474292945,3.0266363174,0.
Fe,3.4948585862,0.0000000017,0.
S,-0.0000000018,3.7457822499,1.3554584688
S,-0.000000001,2.0406523242,-1.2094359598
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H,4.6541148126,3.7095187472,-1.9911778789
H,5.222806534,3.0153887616,-0.4583260798

$[Ru(SMe)_2(CO)_2]_6$

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$[Os(SMe)_2(CO)_2]_6$
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S,-0.0000000013,2.1529644277,1.25844998
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S,-3.3825747308,1.9529304287,1.43089503
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O,-5.821782838,-1.2872802739,1.7562281
O,-5.8217828396,1.287280267,-1.7562281
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H,-5.3595997794,3.0943663711,0.57247005
C,-2.4427560908,-1.4103258886,2.94788498
H,-3.385826219,-1.9548076817,2.98060697
H,-1.671867,-1.99247806,3.45499196
H,-2.5614701159,-0.4516402668,3.45499196
C,-4.9495398774,-2.8576181845,-1.55363705
H,-5.6615089973,-2.2419359668,-2.10582204
H,-4.772327995,-3.7820426378,-2.10582204
H,-5.3595997757,-3.0943663775,-0.57247005
C,0.0000000034,-5.7152363631,1.55363705
H,0.889181005,-6.0239785978,2.10582204
H,-0.8891809978,-6.0239785988,2.10582204
H,0.0000000037,-6.1887327486,0.57247005
C,0.0000000017,-2.8206517742,-2.94788498
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H,0.8896031164,-2.4441183237,-3.45499196
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H,5.3595997794,-3.0943663711,-0.57247005
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H,-0.889181005,6.0239785978,-2.10582204
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C,-0.0000000017,2.8206517742,2.94788498
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C,-2.4427560925,1.4103258856,-2.94788498
H,-2.5614701164,0.4516402637,-3.45499196
H,-3.3858262214,1.9548076776,-2.98060697
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$[Ru(SMe)_2(CO)_2]_8$
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S,0.,3.178561837,1.1554529028
S,0.,4.8498199645,-1.5177439412
S,-2.2475826294,2.2475826294,-1.1554529028
S,-3.4293405844,3.4293405844,1.5177439412
S,-3.178561837,0.,1.1554529028
S,-4.8498199645,0.,-1.5177439412
S,-2.2475826294,-2.2475826294,-1.1554529028
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S,0.,-4.8498199645,-1.5177439412
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O,-3.7500544362,5.9188139632,-1.7464065621
O,-6.8369224116,1.5335445683,1.7464065621
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O,-6.8369224116,-1.5335445683,1.7464065621
O,-5.9188139632,-3.7500544362,-1.7464065621
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C,-1.5941065162,5.9115863751,1.0703199545
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C,-4.6830395514,4.6830395514,1.9043589732
H,-5.4780594789,4.2140965904,2.5013719528
H,-4.2140965904,5.4780594789,2.5013719528
H,-5.1200349224,5.1200349224,0.9954873288
C,-3.6679962262,0.,2.9040470163
H,-4.7568407263,0.,3.0496831748
H,-3.2403654445,-0.897205712,3.3726525023
H,-3.2403654445,0.897205712,3.3726525023
C,-4.6830395514,-4.6830395514,1.9043589732
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H,4.2140965904,-5.4780594789,2.5013719528
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C,3.6679962262,0.,2.9040470163
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H,3.2403654445,-0.897205712,3.3726525023
C,4.6830395514,4.6830395514,1.9043589732
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H,5.4780594789,4.2140965904,2.5013719528
H,5.1200349224,5.1200349224,0.9954873288
C,0.,3.6679962262,2.9040470163
H,0.,4.7568407263,3.0496831748
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H,0.897205712,3.2403654445,3.3726525023
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H,7.240822827,0.,-0.9954873288
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H,6.8533892809,0.8937567296,-2.5013719528
C,2.5936650049,2.5936650049,-2.9040470163
H,1.6568641363,2.9257046224,-3.3726525023
H,3.3635943346,3.3635943346,-3.0496831748
H,2.9257046224,1.6568641363,-3.3726525023
C,0.,6.6228180468,-1.9043589732
H,0.8937567296,6.8533892809,-2.5013719528
H,-0.8937567296,6.8533892809,-2.5013719528
H,0.,7.240822827,-0.9954873288
C,-6.6228180468,0.,-1.9043589732
H,-6.8533892809,0.8937567296,-2.5013719528
H,-6.8533892809,-0.8937567296,-2.5013719528
H,-7.240822827,0.,-0.9954873288
C,-2.5936650049,-2.5936650049,-2.9040470163
H,-1.6568641363,-2.9257046224,-3.3726525023
H,-3.3635943346,-3.3635943346,-3.0496831748
H,-2.9257046224,-1.6568641363,-3.3726525023
C,2.5936650049,-2.5936650049,-2.9040470163
H,2.9257046224,-1.6568641363,-3.3726525023
H,3.3635943346,-3.3635943346,-3.0496831748
H,1.6568641363,-2.9257046224,-3.3726525023
C,0.,-6.6228180468,-1.9043589732
H,0.,-7.240822827,-0.9954873288
H,-0.8937567296,-6.8533892809,-2.5013719528
H,0.8937567296,-6.8533892809,-2.5013719528
C,-2.5936650049,2.5936650049,-2.9040470163
H,-2.9257046224,1.6568641363,-3.3726525023
H,-3.3635943346,3.3635943346,-3.0496831748
H,-1.6568641363,2.9257046224,-3.3726525023

$[Ru(SMe)_2(CO)_2]_{10}$

E = -11968.3218447 a.u.

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Ru,1.8274177452,5.62421351,0.
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S,0.,-4.3279865774,1.09454642
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S,-5.6333212593,1.8303770323,1.5506888226
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S,-2.5439266823,3.5014146925,1.09454642
S,0.,4.3279865774,-1.09454642
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S,3.4815840078,4.7919892829,-1.5506888226
C,5.4107888892,-4.8635383888,-1.0718726666
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C,-7.2361363032,-0.754303297,1.0718726666

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C,1.5187040254,-7.1150671217,1.0718726666
C,-2.9534741572,-6.6488820463,-1.0718726666
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C,-5.4107888892,4.8635383888,1.0718726666
C,-6.2975255967,3.6430500164,-1.0718726666
C,-1.5187040254,7.1150671217,-1.0718726666
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O,5.9088753538,-5.6339732916,-1.7617871794
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O,-8.0919469914,-1.0848303482,1.7617871794
O,-7.1841699136,-3.8786809162,1.7617871794
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C,4.496095602,1.4608700172,-2.8655735291
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H,3.7915960116,2.1752206604,-3.3136284706
C,0.,4.727474682,-2.8655735291
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H,0.89709018,4.2782022445,-3.3136284706
C,-4.496095602,1.4608700172,-2.8655735291
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C,-2.7787398987,3.8246073582,2.8655735291
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H,-3.2404253868,2.9338419434,3.3136284706
H,-1.7889029845,3.988434699,3.3136284706
C,-4.496095602,-1.4608700172,2.8655735291
H,-4.3460282338,-0.4688537375,3.3136284706
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$[Ru(SMe)_2(CO)_2]_{12}$

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S,0,5.4790913951,0.,-1.0625011949
S,0,2.7395456976,4.7450323378,-1.0625011949
S,0,-2.7395456976,4.7450323378,-1.0625011949
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C,-2.0533131994,-1.185480929,-2.9393318767
H,-2.9501711864,-1.7032821295,-3.3088087863
H,-2.0536841801,-0.1542134713,-3.3229006658
H,-1.1603948731,-1.7014359362,-3.3229006658
C,-0.0000000005,2.3709618571,-2.9393318767
H,-0.0000000007,3.4065642577,-3.3088087863
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H,-0.8932893071,1.8556494066,-3.3229006658
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H,2.0536841801,0.1542134713,3.3229006658
H,2.9501711864,1.7032821295,3.3088087863
H,1.1603948731,1.7014359362,3.3229006658
C,-4.8633684631,2.8078670899,-1.9986847567
H,-4.5691288943,3.6639640608,-2.6255186202
H,-5.4576504033,2.1249996629,-2.6255186202
H,-5.5070981746,3.1795246119,-1.1899667739
C,4.8633684619,2.8078670921,-1.9986847567
H,5.4576504024,2.1249996652,-2.6255186202
H,4.5691288927,3.6639640628,-2.6255186202
H,5.5070981732,3.1795246144,-1.1899667739
C,-4.3723481324,-4.7582219339,-0.7259544443
C,-3.0994545292,-4.2062715692,-2.5534432928
C,-3.9783039776,-4.8526841503,-3.4121752884
C,-5.1149227427,-5.472885559,-2.8952043213
C,-5.2994469323,-5.4267531592,-1.5163019082
C,-1.9345670027,-6.1656755246,0.7259544443
C,-2.0499826266,-7.3028322499,1.5163019082
C,-2.1821965516,-7.166095814,2.8952043213
C,-2.2133957593,-5.8716543847,3.4121752884
C,-2.0930107675,-4.7873421457,2.5534432928
H,-2.1858385829,-3.7353452054,-2.9195699911
H,-3.7604826335,-4.8645700202,-4.482213177
H,-5.8277325616,-5.9840808051,-3.5462093898
H,-6.1577968141,-5.9047593005,-1.0395879334
H,-2.0347731468,-8.2851881235,1.0395879334
H,-2.2684997112,-8.0390048483,3.5462093898
H,-2.3325998967,-5.6889585022,4.482213177
H,-2.1419845467,-3.760664345,2.9195699911
N,-3.2858892659,-4.130483594,-1.2188521744
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C,-7.3494295613,-1.876079093,-1.5163019082
C,-7.2971192967,-1.6932102573,-2.8952043213
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C,-6.3069151378,1.4074535899,0.7259544443
C,-5.1924652987,0.5810705756,2.5534432928
C,-6.1916997395,1.0189702334,3.4121752884
C,-7.2971192974,1.6932102541,2.8952043213
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H,-8.0962322754,-2.0549240458,-3.5462093898
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H,-4.3278231312,-0.0253191406,-2.9195699911
H,-4.3278231312,0.0253191387,2.9195699911
H,-6.0930825327,0.824388481,4.482213177
H,-8.0962322763,2.0549240423,3.5462093898
H,-8.1925699645,2.3804288221,1.0395879334
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C,-2.2133957619,5.8716543837,-3.4121752884
C,-2.0930107695,4.7873421448,-2.5534432928
C,-4.3723481345,4.758221932,0.7259544443
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C,-3.9783039797,4.8526841486,3.4121752884
C,-5.1149227451,5.4728855568,2.8952043213
C,-5.2994469347,5.4267531569,1.5163019082
H,-2.0347731504,8.2851881226,-1.0395879334
H,-2.2684997147,8.0390048474,-3.5462093898
H,-2.3325998992,5.6889585012,-4.482213177
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H,-3.7604826356,4.8645700186,4.482213177
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H,-6.1577968167,5.9047592978,1.0395879334
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C,2.2133957619,-5.8716543837,3.4121752884
C,2.0930107695,-4.7873421448,2.5534432928
C,4.3723481345,-4.758221932,-0.7259544443
C,3.099454531,-4.2062715678,-2.5534432928
C,3.9783039797,-4.8526841486,-3.4121752884
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C,5.2994469347,-5.4267531569,-1.5163019082
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H,2.2684997147,-8.0390048474,3.5462093898
H,2.3325998992,-5.6889585012,4.482213177
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H,2.1858385845,-3.7353452044,-2.9195699911
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H,6.1577968167,-5.9047592978,-1.0395879334
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H,8.1925699635,2.3804288257,1.0395879334
H,8.0962322754,2.0549240458,3.5462093898
H,6.0930825324,0.8243884837,4.482213177
H,4.3278231312,0.0253191406,2.9195699911
H,4.3278231312,-0.0253191387,-2.9195699911
H,6.0930825327,-0.824388481,-4.482213177
H,8.0962322763,-2.0549240423,-3.5462093898
H,8.1925699645,-2.3804288221,-1.0395879334
N,5.2200483553,-0.7804217813,-1.2188521744
N,5.2200483549,0.7804217836,1.2188521744
C,4.3723481324,4.7582219339,0.7259544443
C,5.2994469323,5.4267531592,1.5163019082
C,5.1149227427,5.472885559,2.8952043213
C,3.9783039776,4.8526841503,3.4121752884
C,3.0994545292,4.2062715692,2.5534432928
C,1.9345670027,6.1656755246,-0.7259544443
C,2.0930107675,4.7873421457,-2.5534432928
C,2.2133957593,5.8716543847,-3.4121752884
C,2.1821965516,7.166095814,-2.8952043213
C,2.0499826266,7.3028322499,-1.5163019082
H,6.1577968141,5.9047593005,1.0395879334
H,5.8277325616,5.9840808051,3.5462093898
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H,2.1858385829,3.7353452054,2.9195699911
H,2.1419845467,3.760664345,-2.9195699911
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H,1.8417579186,-6.2484727141,-0.3552687506
H,4.490457148,-4.7192455002,0.3552687506
H,6.3322150639,1.5292272147,-0.3552687506
H,6.3322150646,-1.5292272119,0.3552687506
H,1.8417579159,6.2484727149,0.3552687506
H,4.490457146,4.7192455022,-0.3552687506
H,-1.8417579186,6.2484727141,0.3552687506
H,-4.490457148,4.7192455002,-0.3552687506
H,-6.3322150646,1.5292272119,-0.3552687506
H,-6.3322150639,-1.5292272147,0.3552687506

H,-4.490457146,-4.7192455022,0.3552687506

H,-1.8417579159,-6.2484727149,-0.3552687506

$[CO_2 \subset \{Ru(SeMe)_2(CO)_2\}_6]$

Ru	3.909919	0.031718	0.090258
Ru	1.946582	-3.406181	0.095429
Ru	-2.022516	-3.453097	0.103723
Se	3.540006	-2.038768	-1.487311
Se	1.644010	-0.947617	1.045749
Se	-0.024860	-4.159459	1.652860
Se	-0.053710	-3.093673	-1.688789
Se	2.546403	1.565056	-1.635699
Se	3.574686	2.082775	1.679201
O	5.554132	-1.412199	2.216773
O	6.536060	0.953159	-1.177536
O	2.574672	-6.144179	-1.108716
O	4.029226	-4.032744	2.232992
O	-2.611268	-6.210971	-1.073291
O	-4.079720	-4.047734	2.278168
C	4.888291	-0.909490	1.402624
C	5.514082	0.630464	-0.716442
C	2.289483	-5.098576	-0.676466
C	3.249732	-3.736086	1.418673
C	-2.352030	-5.154845	-0.651268
C	-3.310693	-3.773290	1.446374
Ru	-3.909653	-0.005700	0.079620
Ru	-1.949400	3.421563	0.112451
Ru	1.974362	3.470428	0.146194
Se	-3.530801	2.038593	1.666224
Se	-2.380771	1.412793	-1.589472
Se	0.017844	4.236111	-1.430144
Se	0.017892	1.970020	1.100203
Se	-1.667570	-1.004514	1.046980
Se	-3.633764	-2.107044	-1.478933
O	-6.421871	1.100495	-1.272293
O	-5.617701	-1.396009	2.194134
O	-1.582299	5.611526	2.208274
O	-4.158077	5.052089	-1.238432
O	1.526332	5.552511	2.335043
O	4.125975	5.275620	-1.061190
C	-5.451668	0.688654	-0.772235
C	-4.941348	-0.906494	1.380283
C	-1.684799	4.768032	1.409939
C	-3.317694	4.415049	-0.739638
C	1.648207	4.753262	1.495305
C	3.311455	4.562540	-0.626181
C	-0.003982	6.243093	-1.204133
H	0.902724	6.635769	-1.676604
H	-0.903054	6.621846	-1.701857
H	-0.020082	6.481703	-0.137297
C	5.331766	3.067336	1.570081
H	5.205780	4.025639	2.084885
H	6.086691	2.449156	2.067276
H	5.587814	3.221864	0.518854
C	5.292506	-3.033142	-1.330568
H	5.170042	-4.001134	-1.827933
H	6.061001	-2.428834	-1.823996
H	5.526011	-3.168075	-0.270817
C	2.005782	-1.138168	3.024765
H	1.141427	-1.654581	3.455875
H	2.923015	-1.706367	3.202804
H	2.098919	-0.123739	3.427638
C	-0.000549	2.409241	3.073047
H	0.920618	1.998197	3.499910
H	-0.047553	3.490644	3.226990
H	-0.885456	1.922303	3.496551
C	3.977644	2.401679	-2.785803
H	3.487765	3.174615	-3.386606
H	4.775585	2.835590	-2.178650
H	4.371598	1.605666	-3.425922
C	-5.283509	3.036598	1.595190
H	-6.037124	2.413001	2.087583
H	-5.144780	3.982505	2.129425
H	-5.551032	3.216494	0.550781
C	-5.392332	-3.077284	-1.265990
H	-6.163666	-2.478568	-1.761855
H	-5.285260	-4.057162	-1.743239
H	-5.609907	-3.186783	-0.200139
C	0.008146	-6.170249	1.508461
H	0.925088	-6.520868	1.993633
H	-0.880626	-6.553250	2.020840
H	-0.002679	-6.449116	0.451800
C	-0.039832	-4.841566	-2.698236
H	-0.027276	-5.695266	-2.016371
H	-0.942839	-4.859103	-3.316565
H	0.857893	-4.839669	-3.324609
C	-2.020842	-1.205617	3.026548

H	-3.018089	-1.619175	3.200762
H	-1.251271	-1.877807	3.421356
H	-1.934880	-0.206141	3.465530
C	-3.641461	2.153690	-2.978138
H	-4.507562	2.634046	-2.516582
H	-3.066026	2.874787	-3.567778
H	-3.952308	1.306465	-3.598171
C	0.119796	-0.105112	-2.747375
O	0.047560	-0.008117	-3.913671
O	0.194668	-0.211323	-1.578384

$[C_2H_6 \subset \{Ru(SeMe)_2(CO)_2\}_6]$

Ru	2.056296	3.561609	0.000000
Ru	4.112592	0.000000	0.000000
Ru	2.056296	-3.561609	0.000000
Se	3.679595	2.124415	-1.537391
Se	2.421449	1.398024	1.731423
Se	3.679595	-2.124415	1.537391
Se	2.421449	-1.398024	-1.731423
Se	0.000000	2.796048	-1.731423
Se	0.000000	4.248831	1.537391
O	4.286887	4.866369	1.603114
O	2.070956	6.145737	-1.603114
O	6.357842	-1.279368	-1.603114
O	6.357842	1.279368	1.603114
O	4.286887	-4.866369	-1.603114
O	2.070956	-6.145737	1.603114
C	3.425382	4.313896	1.041815
C	2.023252	5.123416	-1.041815
C	5.448635	-0.809520	-1.041815
C	5.448635	0.809520	1.041815
C	3.425382	-4.313896	-1.041815
C	2.023252	-5.123416	1.041815
Ru	-2.056296	-3.561609	0.000000
Ru	-4.112592	0.000000	0.000000
Ru	-2.056296	3.561609	0.000000
Se	-3.679595	-2.124415	1.537391
Se	-2.421449	-1.398024	-1.731423
Se	-3.679595	2.124415	-1.537391
Se	-2.421449	1.398024	1.731423
Se	0.000000	-2.796048	1.731423
Se	0.000000	-4.248831	-1.537391
O	-4.286887	-4.866369	-1.603114
O	-2.070956	-6.145737	1.603114
O	-6.357842	1.279368	1.603114
O	-6.357842	-1.279368	-1.603114
O	-4.286887	4.866369	1.603114
O	-2.070956	6.145737	-1.603114
C	-3.425382	-4.313896	-1.041815
C	-2.023252	-5.123416	1.041815
C	-5.448635	0.809520	1.041815
C	-5.448635	-0.809520	-1.041815
C	-3.425382	4.313896	1.041815
C	-2.023252	5.123416	-1.041815
C	-5.426536	3.133012	-1.440533
H	-5.279355	4.091319	-1.949694
H	-6.182863	2.526396	-1.949694
H	-5.693228	3.286987	-0.391940
C	0.000000	6.266024	1.440533
H	-0.903508	6.617715	1.949694
H	0.903508	6.617715	1.949694
H	0.000000	6.573973	0.391940
C	5.426536	3.133012	-1.440533
H	6.182863	2.526396	-1.949694
H	5.279355	4.091319	-1.949694
H	5.693228	3.286987	-0.391940
C	3.659935	2.113064	3.160834
H	3.956447	1.244562	3.757887
H	4.539676	2.620983	2.763569
H	3.056046	2.804103	3.757887
C	-3.659935	2.113064	3.160834
H	-3.056046	2.804103	3.757887
H	-4.539676	2.620983	2.763569
H	-3.956447	1.244562	3.757887
C	0.000000	4.226128	-3.160834
H	-0.900402	4.048665	-3.757887
H	0.000000	5.241967	-2.763569
H	0.900402	4.048665	-3.757887
C	-5.426536	-3.133012	1.440533
H	-5.279355	-4.091319	1.949694
H	-6.182863	-2.526396	1.949694
H	-5.693228	-3.286987	0.391940
C	0.000000	-6.266024	-1.440533
H	-0.903508	-6.617715	-1.949694
H	0.903508	-6.617715	-1.949694
H	0.000000	-6.573973	-0.391940
C	5.426536	-3.133012	1.440533
H	6.182863	-2.526396	1.949694

H	5.279355	-4.091319	1.949694
H	5.693228	-3.286987	0.391940
C	3.659935	-2.113064	-3.160834
H	4.539676	-2.620983	-2.763569
H	3.056046	-2.804103	-3.757887
H	3.956447	-1.244562	-3.757887
C	0.000000	-4.226128	3.160834
H	0.000000	-5.241967	2.763569
H	0.900402	-4.048665	3.757887
H	-0.900402	-4.048665	3.757887
C	-3.659935	-2.113064	-3.160834
H	-4.539676	-2.620983	-2.763569
H	-3.956447	-1.244562	-3.757887
H	-3.056046	-2.804103	-3.757887
C	0.000000	0.000000	0.746549
H	0.000000	1.017348	1.143667
H	-0.881049	-0.508674	1.143667
C	0.000000	0.000000	-0.746549
H	0.000000	-1.017348	-1.143667
H	-0.881049	0.508674	-1.143667
H	0.881049	-0.508674	1.143667
H	0.881049	0.508674	-1.143667

$[Li\subset[Ru(SMe)_2(CO)_2]_6]^+$

E = -7188.4511088 a.u.

Ru,1.8603615276,3.2222406938,0.
Ru,-1.8603615341,3.22224069,0.
Ru,3.7207230617,0.0000000038,0.
S,-0.000000004,3.9237889221,1.3987059603
S,-0.0000000022,2.1725941999,-1.2202145288
S,1.8815217681,1.0862971019,1.2202145288
S,3.3981008836,1.9618944645,-1.3987059603
S,-3.3981008876,1.9618944576,-1.3987059603
S,-1.8815217703,1.0862970981,1.2202145288
O,3.9953270244,4.3753338209,1.7866587593
O,1.7914867153,5.6477216136,-1.7866587593
O,-1.7914867268,5.64772161,-1.7866587593
O,-3.9953270332,4.3753338128,1.7866587593
O,5.7868137486,1.2723878008,1.7866587593
O,5.7868137512,-1.2723877891,-1.7866587593
C,3.1890887445,3.9384199251,1.1029785778
C,1.8162273241,4.7310418339,-1.1029785778
C,-1.8162273337,4.7310418302,-1.1029785778
C,-3.1890887524,3.9384199187,1.1029785778
C,5.0053160765,0.7926219152,1.1029785778
C,5.0053160782,-0.7926219051,-1.1029785778
Ru,-1.8603615276,-3.2222406938,0.
Ru,1.8603615341,-3.22224069,0.
Ru,-3.7207230617,-0.0000000038,0.
S,0.000000004,-3.9237889221,-1.3987059603
S,0.0000000022,-2.1725941999,1.2202145288
S,-1.8815217681,-1.0862971019,-1.2202145288
S,-3.3981008836,-1.9618944645,1.3987059603
S,3.3981008876,-1.9618944576,1.3987059603
S,1.8815217703,-1.0862970981,-1.2202145288
O,-3.9953270244,-4.3753338209,-1.7866587593
O,-1.7914867153,-5.6477216136,1.7866587593
O,1.7914867268,-5.64772161,1.7866587593
O,3.9953270332,-4.3753338128,-1.7866587593
O,-5.7868137486,-1.2723878008,-1.7866587593
O,-5.7868137512,1.2723877891,1.7866587593
C,-3.1890887445,-3.9384199251,-1.1029785778
C,-1.8162273241,-4.7310418339,1.1029785778
C,1.8162273337,-4.7310418302,1.1029785778
C,3.1890887524,-3.9384199187,-1.1029785778
C,-5.0053160765,-0.7926219152,-1.1029785778
C,-5.0053160782,0.7926219051,1.1029785778
C,-0.0000000058,5.7296187056,1.5706876613
H,-0.8935259053,6.0238141073,2.1388355713
H,0.8935258932,6.0238141091,2.1388355713
H,-0.0000000063,6.2414654002,0.5989953524
C,4.9619953559,-2.8648093478,1.5706876613
H,5.6635389973,-2.2380909207,2.1388355713
H,4.7700130996,-3.785723177,2.1388355713
H,5.4052675966,-3.1207326946,0.5989953524
C,0.0000000058,-5.7296187056,-1.5706876613
H,-0.8935258932,-6.0238141091,-2.1388355713
H,0.8935259053,-6.0238141073,-2.1388355713
H,0.0000000063,-6.2414654002,-0.5989953524
C,2.2311697836,-1.2881664722,-2.9837180591
H,3.1717040399,-1.8311841769,-3.1446188251
H,1.4019868534,-1.849148075,-3.4348822673
H,2.3024026356,-0.2895821887,-3.4348822673
C,-4.9619953501,-2.8648093578,1.5706876613
H,-4.7700130919,-3.7857231866,2.1388355713
H,-5.6635389928,-2.2380909322,2.1388355713
H,-5.4052675902,-3.1207327056,0.5989953524
C,-2.2311697836,1.2881664722,2.9837180591

H,-1.4019868534,1.849148075,3.4348822673
H,-3.1717040399,1.8311841769,3.1446188251
H,-2.3024026356,0.2895821887,3.4348822673
C,0.0000000026,-2.5763329489,2.9837180591
H,-0.9004157816,-2.1387302683,3.4348822673
H,0.0000000037,-3.6623683603,3.1446188251
H,0.9004157859,-2.1387302665,3.4348822673
C,-2.231169781,-1.2881664767,-2.9837180591
H,-3.1717040362,-1.8311841834,-3.1446188251
H,-2.302402635,-0.2895821933,-3.4348822673
H,-1.4019868497,-1.8491480779,-3.4348822673
C,-0.0000000026,2.5763329489,-2.9837180591
H,-0.0000000037,3.6623683603,-3.1446188251
H,0.9004157816,2.1387302683,-3.4348822673
H,-0.9004157859,2.1387302665,-3.4348822673
C,2.231169781,1.2881664767,2.9837180591
H,2.302402635,0.2895821933,3.4348822673
H,3.1717040362,1.8311841834,3.1446188251
H,1.4019868497,1.8491480779,3.4348822673
C,-4.9619953559,2.8648093478,-1.5706876613
H,-4.7700130996,3.785723177,-2.1388355713
H,-5.6635389973,2.2380909207,-2.1388355713
H,-5.4052675966,3.1207326946,-0.5989953524
C,4.9619953501,2.8648093578,-1.5706876613
H,5.6635389928,2.2380909322,-2.1388355713
H,4.7700130919,3.7857231866,-2.1388355713
H,5.4052675902,3.1207327056,-0.5989953524
Li,0.,0.,0.

$[Na\subset[Ru(SMe)_2(CO)_2]_6]^+$

E = -7343.0660511 a.u.

Ru,1.8838409752,3.2623386922,-0.0004137201
Ru,-1.8835404777,3.2618018082,-0.0000224575
Ru,3.7679385605,0.0002595615,0.0005989612
S,0.0001849738,3.9517886027,1.3893627419
S,-0.0000043934,2.310693491,-1.2881365435
S,1.9788212556,1.1433007383,1.2658305235
S,3.4269411217,1.9765794039,-1.39063511
S,-3.4260005714,1.9756240241,-1.3900491994
S,-1.9781450256,1.1428857084,1.2664040107
O,4.014428896,4.415044194,1.7888194068
O,1.839019839,5.7041487137,-1.7623338201
O,-1.8396253197,5.7032010033,-1.762623648
O,-4.0141556455,4.4145460364,1.789198788
O,5.8312850799,1.2754358395,1.7852252704
O,5.8612934524,-1.2638604417,-1.7568267808
C,3.2096104845,3.9714102119,1.1074511371
C,1.8489805446,4.777456241,-1.0917198046
C,-1.8492347187,4.7766826867,-1.0917617244
C,-3.2093287282,3.9708832283,1.1078581453
C,5.0445536824,0.7975001196,1.1061175035
C,5.0634165788,-0.7896580229,-1.0880559648
Ru,-1.883669783,-3.2617417866,-0.0004654995
Ru,1.8832160237,-3.2612940912,-0.0009852576
Ru,-3.7679269628,-0.0001897173,0.0016718533
S,-0.0003150641,-3.9506976408,-1.3921961425
S,-0.0000703931,-2.2845148003,1.266861131
S,-2.0018200113,-1.1550146629,-1.2861577876
S,-3.4242279659,-1.9762040745,1.3916895728
S,3.4233397227,-1.9753969215,1.3909070887
S,2.0012898262,-1.1547278798,-1.2868067536
O,-4.019448733,-4.444141155,-1.7637772255
O,-1.8087721602,-5.6875519225,1.7825029204
O,1.8090596367,-5.6866314839,1.7827022102
O,4.0186523246,-4.4440026888,-1.7645363425
O,-5.861358384,-1.2637165628,-1.7561304463
O,-5.8309099258,1.2765387565,1.7855607967
C,-3.2121233242,-3.9897536017,-1.0927723682
C,-1.8303803373,-4.766825605,1.1038721358
C,1.8303696282,-4.7660943166,1.1038044618
C,3.2114592624,-3.9894885223,-1.0934573966
C,-5.063468324,-0.7897494254,-1.0872064101
C,-5.0443494242,0.797920642,1.1067355671
C,-0.000102411,5.7563010345,1.5732445995
H,-0.8931856608,6.0473095494,2.1436783134
H,0.8937429948,6.0477031321,2.1422794157
H,-0.000974915,6.2734012356,0.6044393632
C,4.9852830341,-2.8786349975,1.5782566201
H,5.6841744454,-2.248917875,2.1461620205
H,4.7894221891,-3.7956799966,2.1512408649
H,5.4338196134,-3.1414529405,0.6106994705
C,-0.0000707368,-5.7553894334,-1.5752349442
H,-0.8940073857,-6.0470414162,-2.1442520258
H,0.8930328104,-6.0466892653,-2.1457404731
H,0.0008396316,-6.2719960624,-0.606436647
C,2.4520493534,-1.4145354907,-3.0188117746
H,3.402126948,-1.9553287965,-3.1197293504
H,1.6472105887,-1.9916376592,-3.4932947106

H,2.5365219824,-0.4290320073,-3.4957840636
C,-4.9866872391,-2.8791082896,1.5768090364
H,-4.7914478071,-3.7976631169,2.1475847738
H,-5.6853474542,-2.2504256061,2.1461818918
H,-5.4353654169,-3.1392904088,0.6085106322
C,-2.3986493628,1.3857533867,3.0083940938
H,-1.5829476513,1.9530370993,3.4761256301
H,-3.3436417173,1.9307389479,3.1312095095
H,-2.481640351,0.3954805991,3.4758330568
C,0.0002711053,-2.7730130381,3.0080039032
H,-0.8992628696,-2.3512536714,3.4758677055
H,0.0009339857,-3.8642031423,3.1291433323
H,0.8993154569,-2.3501929419,3.4758620805
C,-2.4531819372,-1.4151412091,-3.017986805
H,-3.4026866785,-1.9570211198,-3.1184826069
H,-2.5390521238,-0.4297290847,-3.4948362732
H,-1.6479309194,-1.9913058035,-3.4929352376
C,-0.0002326657,2.8292012923,-3.0205014202
H,-0.0014068051,3.9223613487,-3.1225774336
H,0.8994510713,2.4154507094,-3.4951437994
H,-0.8987537818,2.4134447201,-3.4956020646
C,2.4000821508,1.3863012319,3.007646826
H,2.4835925157,0.396061717,3.4750150253
H,3.3450321825,1.9314747114,3.1299757274
H,1.5845024305,1.9534006685,3.4758625411
C,-4.9883249354,2.8791305474,-1.5734225175
H,-4.793787995,3.7960673294,-2.1472924283
H,-5.6888278683,2.2493976146,-2.1395733901
H,-5.4342720577,3.1421485635,-0.6049654261
C,4.9897613,2.8798372823,-1.5714748708
H,5.6901497838,2.2512559293,-2.1390850248
H,4.7958650385,3.7983436519,-2.1430515051
H,5.4356993801,3.1401300582,-0.6021782631
Na,0.0000825611,0.0001666325,-0.0417372007

$[K\subset[Ru(SMe)_2(CO)_2]_6]^+$

E = -7780.5640843 a.u.

Ru,1.9084937946,3.3013915277,-0.0036278665
Ru,-1.9084937831,3.3013915343,-0.0036278665
Ru,3.81951579,-0.0000000067,0.
S,0.0000000069,3.9810871138,1.3712359757
S,0.0000000043,2.4491488012,-1.3832991414
S,2.1266514316,1.225209585,1.377066185
S,3.4610739586,1.9931325103,-1.3772101391
S,-3.4610739517,1.9931325224,-1.3772101391
S,-2.1266514273,1.2252095924,1.377066185
O,4.0378731258,4.510744453,1.7415860087
O,1.8764450718,5.7495038651,-1.7499844528
O,-1.8764450517,5.7495038716,-1.7499844528
O,-4.0378731101,4.510744467,1.7415860087
O,5.9268838015,1.25719534,1.7381889199
O,5.9268837971,-1.2571953607,-1.7381889199
C,3.2311342991,4.0334738504,1.0853343362
C,1.873038134,4.8125087396,-1.0932926288
C,-1.8730381172,4.8125087461,-1.0932926288
C,-3.2311342851,4.0334738616,1.0853343362
C,5.1124461398,0.7884042146,1.0853752397
C,5.112446137,-0.7884042324,-1.0853752397
Ru,-1.9084937946,-3.3013915277,0.0036278665
Ru,1.9084937831,-3.3013915343,0.0036278665
Ru,-3.81951579,0.0000000067,0.
S,-0.0000000069,-3.9810871138,-1.3712359757
S,-0.0000000043,-2.4491488012,1.3832991414
S,-2.1266514316,-1.225209585,-1.377066185
S,-3.4610739586,-1.9931325103,1.3772101391
S,3.4610739517,-1.9931325224,1.3772101391
S,2.1266514273,-1.2252095924,-1.377066185
O,-4.0378731258,-4.510744453,-1.7415860087
O,-1.8764450718,-5.7495038651,1.7499844528
O,1.8764450517,-5.7495038716,1.7499844528
O,4.0378731101,-4.510744467,-1.7415860087
O,-5.9268838015,-1.25719534,-1.7381889199
O,-5.9268837971,1.2571953607,1.7381889199
C,-3.2311342991,-4.0334738504,-1.0853343362
C,-1.873038134,-4.8125087396,1.0932926288
C,1.8730381172,-4.8125087461,1.0932926288
C,3.2311342851,-4.0334738616,-1.0853343362
C,-5.1124461398,-0.7884042146,-1.0853752397
C,-5.112446137,0.7884042324,1.0853752397
C,0.0000000101,5.7851981748,1.563813119
H,-0.8933800846,6.0735977272,2.1351743965
H,0.8933801058,6.0735977241,2.1351743965
H,0.000000011,6.3078324861,0.598019366
C,5.0230493278,-2.8986559349,1.5604155102
H,5.7241525465,-2.2699362209,2.1268526487
H,4.8274452386,-3.8155385392,2.1338473929
H,5.4695149086,-3.1621508925,0.5920980825
C,-0.0000000101,-5.7851981748,-1.563813119

H,-0.8933801058,-6.0735977241,-2.1351743965
H,0.8933800846,-6.0735977272,-2.1351743965
H,-0.000000011,-6.3078324861,-0.598019366
C,2.7333727129,-1.5756932115,-3.0451349043
H,3.6815358284,-2.1282033529,-3.0501267664
H,1.9617421135,-2.1628442966,-3.5609828533
H,2.8646435333,-0.6128672706,-3.5570031856
C,-5.0230493379,-2.8986559174,1.5604155102
H,-4.8274452519,-3.8155385224,2.1338473929
H,-5.7241525544,-2.269936201,2.1268526487
H,-5.4695149196,-3.1621508735,0.5920980825
C,-2.7333727129,1.5756932115,3.0451349043
H,-1.9617421135,2.1628442966,3.5609828533
H,-3.6815358284,2.1282033529,3.0501267664
H,-2.8646435333,0.6128672706,3.5570031856
C,-0.0000000055,-3.1446496848,3.0532266537
H,-0.8969412311,-2.7712940569,3.5653694028
H,-0.0000000074,-4.2419521758,3.0620524183
H,0.8969412215,-2.77129406,3.5653694028
C,-2.7333727184,-1.575693202,-3.0451349043
H,-3.6815358358,-2.12820334,-3.0501267664
H,-2.8646435355,-0.6128672606,-3.5570031856
H,-1.961742121,-2.1628442898,-3.5609828533
C,0.0000000055,3.1446496848,-3.0532266537
H,0.0000000074,4.2419521758,-3.0620524183
H,0.8969412311,2.7712940569,-3.5653694028
H,-0.8969412215,2.77129406,-3.5653694028
C,2.7333727184,1.575693202,3.0451349043
H,2.8646435355,0.6128672606,3.5570031856
H,3.6815358358,2.12820334,3.0501267664
H,1.961742121,2.1628442898,3.5609828533
C,-5.0230493278,2.8986559349,-1.5604155102
H,-4.8274452386,3.8155385392,-2.1338473929
H,-5.7241525465,2.2699362209,-2.1268526487
H,-5.4695149086,3.1621508925,-0.5920980825
C,5.0230493379,2.8986559174,-1.5604155102
H,5.7241525544,2.269936201,-2.1268526487
H,4.8274452519,3.8155385224,-2.1338473929
H,5.4695149196,3.1621508735,-0.5920980825
K,0.,0.,0.

$[Na\subset[Ru(SMe)_2(CO)_2]_8]^+$

E = -9736.7627369 a.u.

Ru,1.8085189916,4.3661510774,0.
Ru,-1.8085189916,4.3661510774,0.
Ru,-4.3661510774,1.8085189916,0.
Ru,-4.3661510774,-1.8085189916,0.
Ru,-1.8085189916,-4.3661510774,0.
Ru,1.8085189916,-4.3661510774,0.
Ru,4.3661510774,-1.8085189916,0.
Ru,4.3661510774,1.8085189916,0.
S,2.2044739942,2.2044739942,-1.1550820249
S,3.4150010256,3.4150010256,1.524918346
S,0.,3.1175970205,1.1550820249
S,0.,4.8295407659,-1.524918346
S,-2.2044739942,2.2044739942,-1.1550820249
S,-3.4150010256,3.4150010256,1.524918346
S,-3.1175970205,0.,1.1550820249
S,-4.8295407659,0.,-1.524918346
S,-2.2044739942,-2.2044739942,-1.1550820249
S,-3.4150010256,-3.4150010256,1.524918346
S,0.,-3.1175970205,1.1550820249
S,0.,-4.8295407659,-1.524918346
S,2.2044739942,-2.2044739942,-1.1550820249
S,3.4150010256,-3.4150010256,1.524918346
S,3.1175970205,0.,1.1550820249
S,4.8295407659,0.,-1.524918346
O,1.5244303122,6.8021422111,1.7433248733
O,3.7319058728,5.8877758953,-1.7433248733
O,-1.5244303122,6.8021422111,1.7433248733
O,-3.7319058728,5.8877758953,-1.7433248733
O,-6.8021422111,1.5244303122,1.7433248733
O,-5.8877758953,3.7319058728,-1.7433248733
O,-6.8021422111,-1.5244303122,1.7433248733
O,-5.8877758953,-3.7319058728,-1.7433248733
C,1.5891191018,5.8791012075,1.0690988761
C,3.0334754381,5.2808292241,-1.0690988761
C,-1.5891191018,5.8791012075,1.0690988761
C,-3.0334754381,5.2808292241,-1.0690988761
C,-5.8791012075,1.5891191018,1.0690988761
C,-5.2808292241,3.0334754381,-1.0690988761
C,-5.8791012075,-1.5891191018,1.0690988761
C,-5.2808292241,-3.0334754381,-1.0690988761
O,-1.5244303122,-6.8021422111,1.7433248733
O,-3.7319058728,-5.8877758953,-1.7433248733
O,1.5244303122,-6.8021422111,1.7433248733
O,3.7319058728,-5.8877758953,-1.7433248733
O,6.8021422111,-1.5244303122,1.7433248733

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O,6.8021422111,1.5244303122,1.7433248733
O,5.8877758953,3.7319058728,-1.7433248733
C,-1.5891191018,-5.8791012075,1.0690988761
C,-3.0334754381,-5.2808292241,-1.0690988761
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C,3.0334754381,-5.2808292241,-1.0690988761
C,5.8791012075,-1.5891191018,1.0690988761
C,5.2808292241,-3.0334754381,-1.0690988761
C,5.8791012075,1.5891191018,1.0690988761
C,5.2808292241,3.0334754381,-1.0690988761
C,-4.6689813595,4.6689813595,1.9113540068
H,-5.4621274026,4.1995796796,2.5099634973
H,-4.1995796796,5.4621274026,2.5099634973
H,-5.1068281231,5.1068281231,1.0036763702
C,-3.5499885597,0.,2.9188062292
H,-4.6368653396,0.,3.0748145944
H,-3.1184825231,-0.8993670818,3.3784309086
H,-3.1184825231,0.8993670818,3.3784309086
C,-4.6689813595,-4.6689813595,1.9113540068
H,-4.1995796796,-5.4621274026,2.5099634973
H,-5.4621274026,-4.1995796796,2.5099634973
H,-5.1068281231,-5.1068281231,1.0036763702
C,0.,-3.5499885597,2.9188062292
H,0.,-4.6368653396,3.0748145944
H,0.8993670818,-3.1184825231,3.3784309086
H,-0.8993670818,-3.1184825231,3.3784309086
C,4.6689813595,-4.6689813595,1.9113540068
H,5.4621274026,-4.1995796796,2.5099634973
H,4.1995796796,-5.4621274026,2.5099634973
H,5.1068281231,-5.1068281231,1.0036763702
C,3.5499885597,0.,2.9188062292
H,4.6368653396,0.,3.0748145944
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C,4.6689813595,4.6689813595,1.9113540068
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H,7.2221455924,0.,-1.0036763702
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C,0.,6.6029367611,-1.9113540068
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H,-0.8927560565,6.8318585956,-2.5099634973
H,0.,7.2221455924,-1.0036763702
C,-6.6029367611,0.,-1.9113540068
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H,-6.8318585956,-0.8927560565,-2.5099634973
H,-7.2221455924,0.,-1.0036763702
C,-2.5102209837,-2.5102209837,-2.9188062292
H,-1.5691515768,-2.8410487014,-3.3784309086
H,-3.278758925,-3.278758925,-3.0748145944
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C,0.,-6.6029367611,-1.9113540068
H,0.,-7.2221455924,-1.0036763702
H,-0.8927560565,-6.8318585956,-2.5099634973
H,0.8927560565,-6.8318585956,-2.5099634973
C,-2.5102209837,2.5102209837,-2.9188062292
H,-2.8410487014,1.5691515768,-3.3784309086
H,-3.278758925,3.278758925,-3.0748145944
H,-1.5691515768,2.8410487014,-3.3784309086
Na,0.,0.,0.

$[K\subset[Ru(SMe)_2(CO)_2]_8]^+$

E = -10174.3240846 a.u.

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C,0,-1.6009274597,5.9170674056,1.0680159399
C,0,-3.0519718243,5.3160251501,-1.0680159399
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H,0,-4.2201316292,5.4828084393,2.5089915136
H,0,-5.1327793163,5.1327793163,1.0047162123
C,0,-3.6381976141,0.,2.9253190704
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C,0,-4.6917778607,-4.6917778607,1.9093548534
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C,0,6.6351758822,0.,-1.9093548534
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H,0,6.8610147199,0.8928473349,-2.5089915136
C,0,2.5725942042,2.5725942042,-2.9253190704
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C,0,0.,6.6351758822,-1.9093548534

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C,0,-6.6351758822,0.,-1.9093548534
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H,0,-6.8610147199,-0.8928473349,-2.5089915136
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H,0,-3.3420945513,3.3420945513,-3.0716813407
H,0,-1.6345127386,2.9062049624,-3.3891650852
K,0,0.,0.,0.

$[Rb\subset[Ru(SMe)_2(CO)_2]_8]^+$

E = -9598.7362021 a.u.

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Ru,-1.8356997749,-4.4317712931,0.
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Ru,4.4317712931,-1.8356997749,0.
Ru,4.4317712931,1.8356997749,0.
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S,3.4579358234,3.4579358234,1.5056618586
S,0.,3.2323488066,1.1741008473
S,0.,4.8902597393,-1.5056618586
S,-2.2856157603,2.2856157603,-1.1741008473
S,-3.4579358234,3.4579358234,1.5056618586
S,-3.2323488066,0.,1.1741008473
S,-4.8902597393,0.,-1.5056618586
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S,3.2323488066,0.,1.1741008473
S,4.8902597393,0.,-1.5056618586
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C,1.6095530393,5.9432933927,1.0685969987
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C,5.3406689293,3.0644171918,-1.0685969987
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H,-4.2368753193,5.4996266767,2.5058377481
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H,-4.7799848393,0.,3.0756430375
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H,-5.4996266767,-4.2368753193,2.5058377481
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H,0.8989746369,3.2644195549,3.3955676477
C,6.6603969296,0.,-1.9057401565
H,7.2862441103,0.,-1.0025902313
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H,6.8847465864,0.8929000478,-2.5058377481
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C,0.,6.6603969296,-1.9057401565
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H,0.,7.2862441103,-1.0025902313
C,-6.6603969296,0.,-1.9057401565
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H,-6.8847465864,-0.8929000478,-2.5058377481
H,-7.2862441103,0.,-1.0025902313
C,-2.6102956991,-2.6102956991,-2.9306553844
H,-1.6726221421,-2.9439642658,-3.3955676477
H,-3.3799596938,-3.3799596938,-3.0756430375
H,-2.9439642658,-1.6726221421,-3.3955676477
C,2.6102956991,-2.6102956991,-2.9306553844
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H,0.,-7.2862441103,-1.0025902313
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H,0.8929000478,-6.8847465864,-2.5058377481
C,-2.6102956991,2.6102956991,-2.9306553844
H,-2.9439642658,1.6726221421,-3.3955676477
H,-3.3799596938,3.3799596938,-3.0756430375
H,-1.6726221421,2.9439642658,-3.3955676477
Rb,0.,0.,0.

$[Cu\subset[Ru(SMe)_2(CO)_2]_6]^+$
E = -8820.9739306 a.u.

Ru,24.375209895,1.8187244007,-0.0121836108
S,25.6291952902,3.3561188783,1.3981202556
S,25.5253113299,-0.0205549796,1.144523884
O,22.0134911559,1.6241781355,1.8440186389
O,23.0693036572,3.9626650541,-1.6873726946
C,22.9092326584,1.6961194263,1.1362162652
C,23.5676976088,3.1531683424,-1.0505013336
Ru,27.6671272315,-3.7150559959,-0.0060776601
S,25.7062258203,-3.4007279891,1.4001075939
S,28.6873176328,-1.7991993204,1.1481171909
O,29.0177106314,-5.6632410011,1.8496193817
O,26.4587257179,-5.9166482394,-1.6801763829
C,28.5068919026,-4.9236038172,1.1421613177
C,26.9141661133,-5.0813961096,-1.044312422
Ru,30.8143329075,1.9038578852,-0.01107376
S,31.5202472519,0.0470387464,1.3946609157
S,28.6442608727,1.8237171867,1.1389536713
O,31.8226970056,4.0463753665,1.8478590965
O,33.3257415955,1.9635629925,-1.6844572971
C,31.4393950643,3.234044528,1.1395026494
C,32.3749407062,1.9373226342,-1.0483794668
Ru,30.8553654432,-1.8233793431,-0.0114402984
S,29.616983528,-3.3726929428,-1.4137371712
S,29.8965793865,0.0311061362,-1.3092320646
O,33.3598321895,-1.8289382608,-1.6960473541

O,31.9364348196,-3.9286082728,1.8501216655
C,32.4120119044,-1.822159935,-1.0550235274
C,31.5222889331,-3.1338698926,1.139258287
Ru,27.5820416322,3.7183950823,-0.010163627
S,29.5435037395,3.4284527091,-1.4144185157
S,26.4576387606,1.9601609072,-1.3076611462
O,26.3346778538,5.8917020116,-1.6926299744
O,28.8612469079,5.6996961069,1.8609876313
C,26.8020480007,5.0675507065,-1.051052199
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$[Ag\subset[Ru(SMe)_2(CO)_2]_6]^+$

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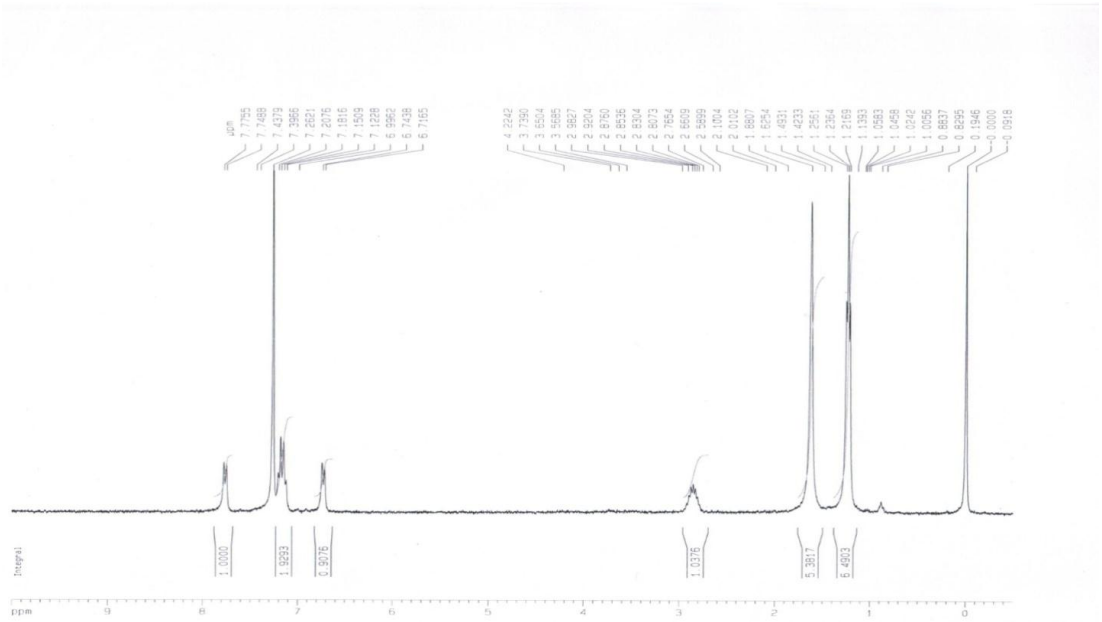

Fig. S2. NMR spectrum of $[Cu(Ru\{S(4\text{-}i\text{Pr-}C_6H_4)\}_2(CO)_2)_6]^+$.

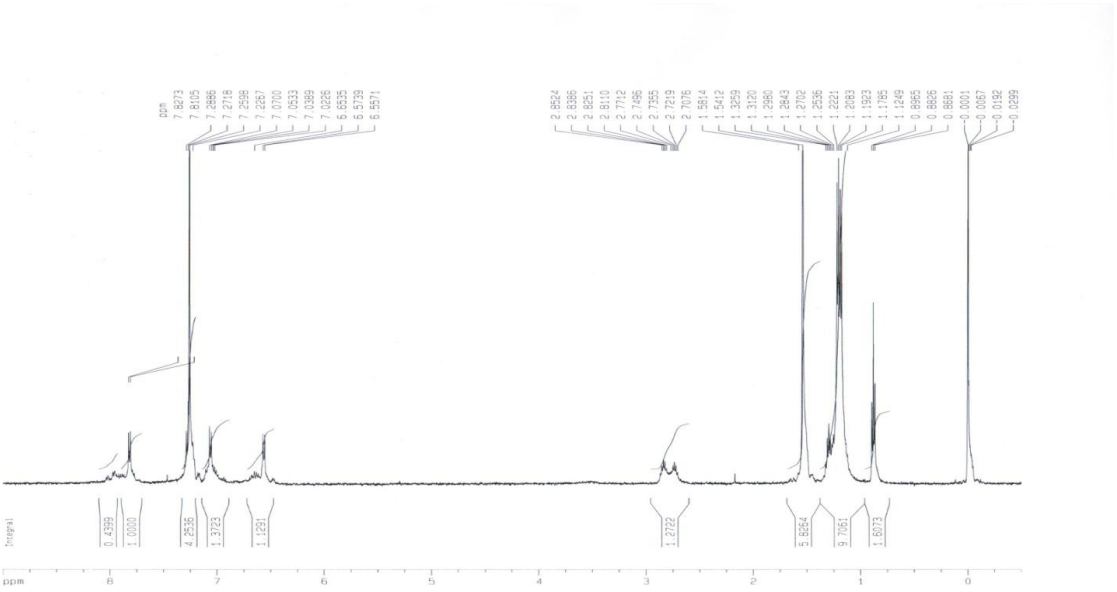

Fig. S3. NMR spectrum of $[K(Ru\{S(4\text{-}i\text{Pr-}C_6H_4)\}_2(CO)_2)_6]^+$.

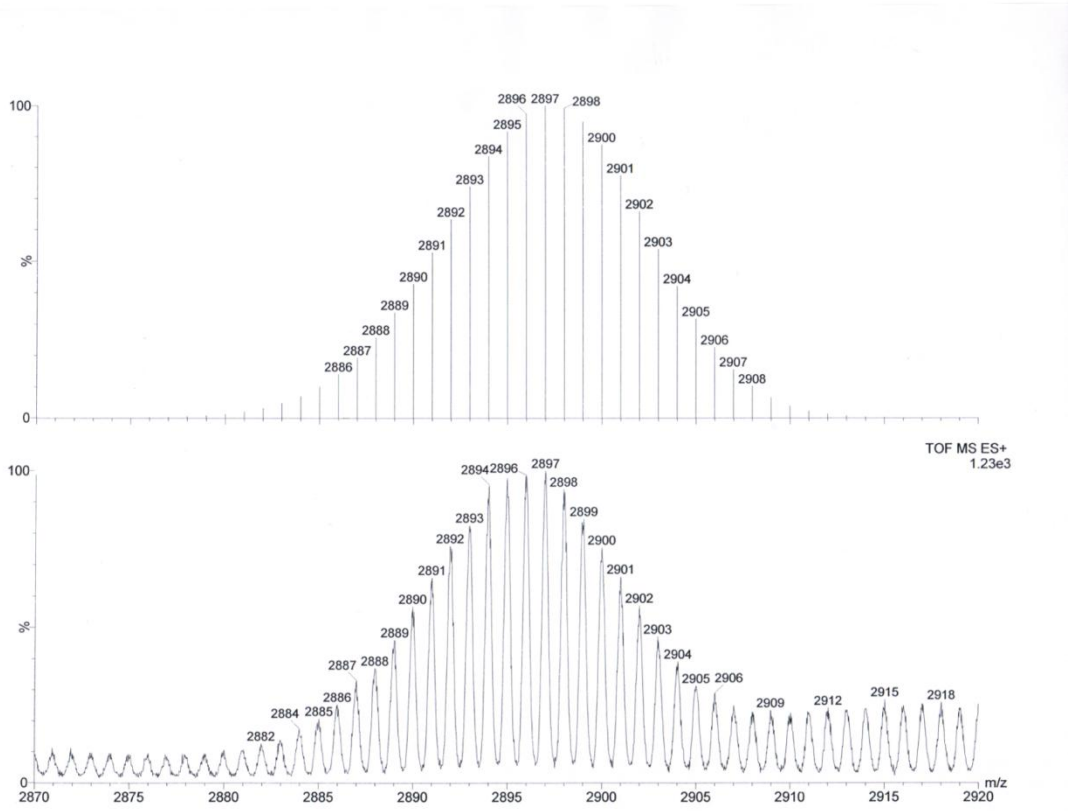

Fig. S4. Top: Simulated pattern of $[K_2HCO_3[Ru\{S(4\text{-}i\text{Pr-Ph})\}_2(CO)_2]_6]$; bottom: electrospray ionization mass spectrometric measurement of $[K_2HCO_3[Ru\{S(4\text{-}i\text{Pr-}C_6H_4)\}_2(CO)_2]_6]$.

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