SUPPLEMENTARY INFORMATION

Cation recognition by benzene sandwich compounds – a DFT perspective

Katarina A. Ćeranić,[a] Snežana D. Zarić,[b] and Dušan P. Malenov[b,*]

[a] *Innovative Centre of the Faculty of Chemistry, Belgrade, Serbia,* [b] *University of Belgrade – Faculty of Chemistry, Belgrade, Serbia*

e-mail: malenov@chem.bg.ac.rs

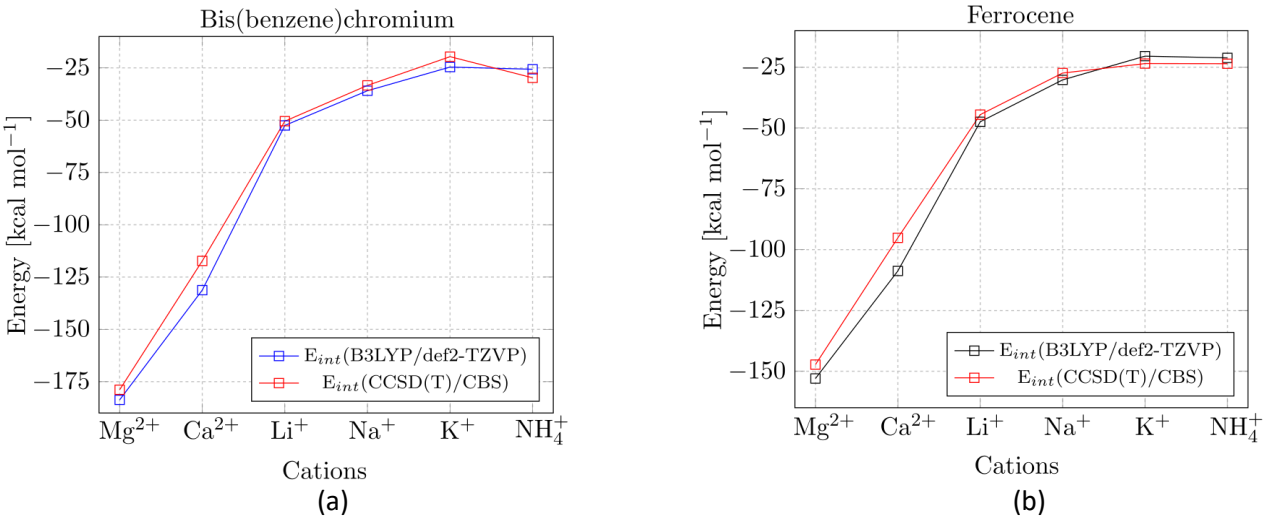


Figure S1. Comparison of interaction energy calculated at the B3LYP/def2-TZVP level, E_{int}(B3LYP/def2-TZVP), and at the CCSDT/CBS level, E_{int}(CCSDT/CBS), for (a) bis(benzene)chromium and (b) ferrocene.

Table S1. Comparison of energies of cation-π interactions obtained using B3LYP method without the dispersion correction and with D3 dispersion correction, with CCSD(T)/CBS energies which serve as reference data

system	cation	E_{int} B3LYP/def2-TZVP [kcal/mol]	E_{int} B3LYP-D3/def2-TZVP [kcal/mol]	E_{int} CCSD(T)/CBS [kcal/mol]
benzene	Mg^{2+}	-121.78	-124.64	-115.50
	Ca^{2+}	-81.88	-84.44	-70.95
	Li^{+}	-38.37	-39.14	-36.83
	Na^{+}	-23.87	-25.39	-22.12
	K^{+}	-15.88	-18.25	-13.13
	NH_4^{+}	-16.22	-20.60	-19.09
bis(benzene)chromium	Mg^{2+}	-183.71	-189.66	-178.87
	Ca^{2+}	-131.25	-136.91	-117.28
	Li^{+}	-52.52	-53.89	-50.47
	Na^{+}	-35.92	-38.59	-33.37
	K^{+}	-24.60	-27.77	-19.64
	NH_4^{+}	-25.67	-30.22	-29.75
ferrocene	Mg^{2+}	-152.98	-156.86	-147.26
	Ca^{2+}	-108.77	-112.31	-95.15
	Li^{+}	-47.44	-49.47	-44.50
	Na^{+}	-30.21	-32.98	-27.40
	K^{+}	-20.46	-23.21	-23.52
	NH_4^{+}	-21.17	-25.13	-23.58

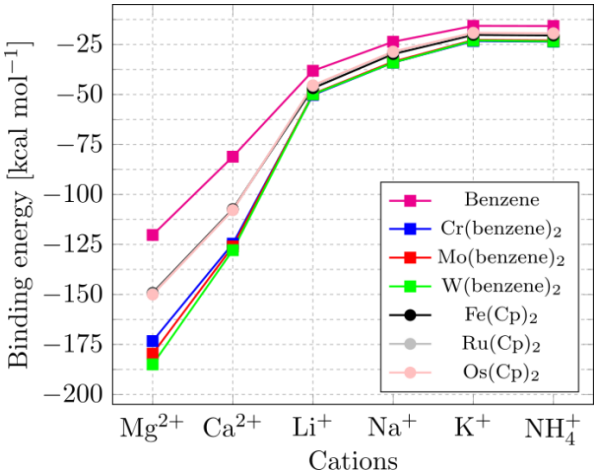


Figure S2. Binding energies for studied cation-π interactions. Calculations were done at the B3LYP/def2-TZVP level.

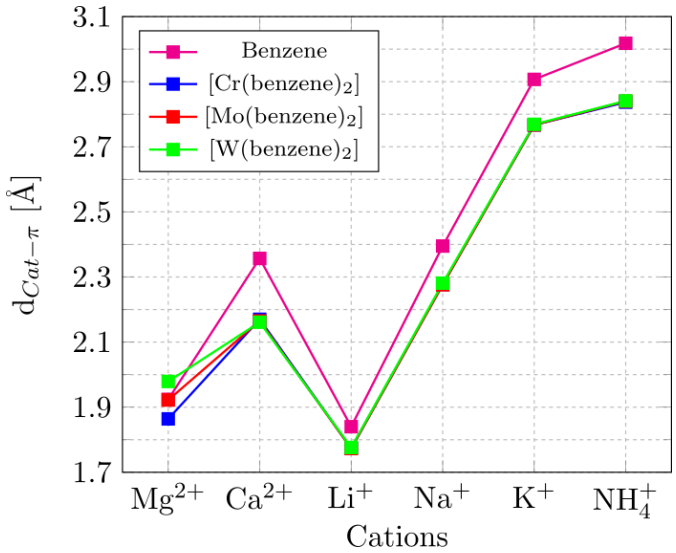


Figure S3. Cation-π distances, $d_{Cat-\pi}$, between cations Mg^{2+}, Ca^{2+}, Li^{+}, Na^{+}, K^{+}, NH_4^{+} and the center of the benzene ring of the corresponding sandwich compounds (for NH_4^{+} it is N-center distance). Calculations were done at the B3LYP/def2-TZVP level.

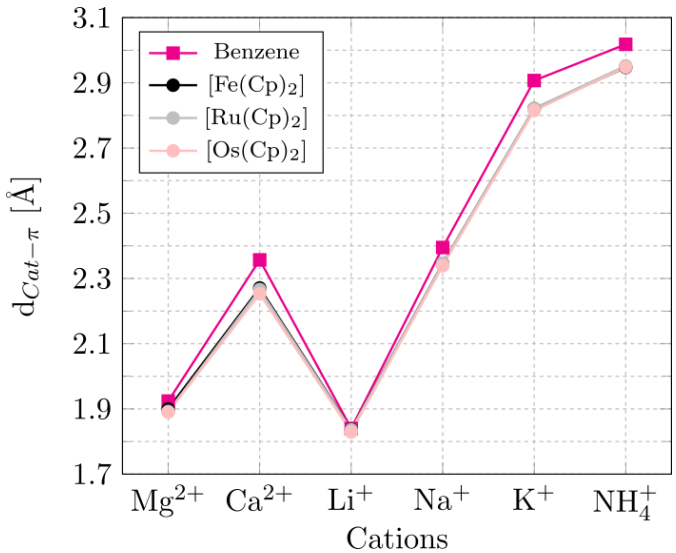


Figure S4. Cation-π distances, $d_{Cat-\pi}$, between cations Mg^{2+}, Ca^{2+}, Li^{+}, Na^{+}, K^{+}, NH_4^{+} and the center of the Cp ring of the corresponding sandwich compounds (for NH_4^{+} it is N-center distance). Calculations were done at the B3LYP/def2-TZVP level.

Table S2. Cation-π distances ($d_{cat-\pi}$), interaction and binding energies (E_{int} and E_{bind}, respectively) calculated at the B3LYP/def2-TZVP level for cation-π interactions of bis(benzene)chromium, bis(benzene)molybdenum and bis(benzene)tungsten. For NH_4^+ the $d_{cat-\pi}$ is N-center distance.

System	Cation	$d_{Cat-\pi}$ (Å)	E_{int} (kcal/mol)	E_{bind} (kcal/mol)
Benzene	**Mg^{2+}**	1.924	-121.78	-120.27
	Ca^{2+}	2.357	-81.88	-81.12
	Li^+	1.840	-38.37	-38.16
	Na^+	2.395	-23.87	-23.64
	K^+	2.907	-15.88	-15.68
	NH_4^+	3.018	-16.22	-15.77
Bis(benzene)chromium	**Mg^{2+}**	1.864	-183.71	-173.33
	Ca^{2+}	2.170	-131.25	-124.58
	Li^+	1.773	-52.52	-50.25
	Na^+	2.277	-35.92	-34.03
	K^+	2.767	-24.60	-23.29
	NH_4^+	2.837	-25.67	-23.60
Bis(benzene)molybdenum	**Mg^{2+}**	1.922	-191.64	-179.63
	Ca^{2+}	2.165	-133.46	-126.02
	Li^+	1.773	-52.30	-49.70
	Na^+	2.276	-35.81	-33.59
	K^+	2.767	-24.20	-22.73
	NH_4^+	2.840	-25.27	-23.02
Bis(benzene)tungsten	**Mg^{2+}**	1.979	-196.77	-184.99
	Ca^{2+}	2.161	-135.53	-127.87
	Li^+	1.776	-52.50	-49.92
	Na^+	2.281	-36.30	-34.05
	K^+	2.769	-24.48	-23.01
	NH_4^+	2.841	-25.74	-23.43

Table S3. Deformation energies of benzene and benzene sandwich compounds (E_{def}), metal-π distances ($d_{M-\pi}$), and average lengths of the carbon-carbon bonds in the benzene aromatic rings interacting with the cations (d_{C-C}) for cation-π interactions of bis(benzene)chromium, bis(benzene)molybdenum and bis(benzene)tungsten. Calculations were done at the B3LYP/def2-TZVP level. In the brackets are the deformation energies of ammonium ion, as well as the changes in $d_{M-\pi}$ and d_{C-C} distances.

System	Cation	E_{def} (kcal/mol)	$d_{M-\pi}$ (Å)	d_{C-C} (Å)
Benzene	Without	0.00	-	1.391
	Mg^{2+}	1.51	-	1.412 (+0.021)
	Ca^{2+}	0.76	-	1.404 (+0.013)
	Li^{+}	0.22	-	1.399 (+0.008)
	Na^{+}	0.23	-	1.397 (+0.006)
	K^{+}	0.20	-	1.395 (+0.004)
	NH_4^{+}	0.19 (0.25)	-	1.395 (+0.004)
Bis(benzene)chromium	Without	0.00	1.651	1.413
	Mg^{2+}	10.38	1.493 (-0.158)	1.447 (+0.034)
	Ca^{2+}	6.67	1.540 (-0.111)	1.439 (+0.026)
	Li^{+}	2.27	1.578 (-0.073)	1.428 (+0.015)
	Na^{+}	1.88	1.580 (-0.071)	1.427 (+0.014)
	K^{+}	1.31	1.593 (-0.058)	1.423 (+0.010)
	NH_4^{+}	1.46 (0.60)	1.591 (-0.060)	1.424 (+0.011)
Bis(benzene)molybdenum	Without	0.00	1.819	1.416
	Mg^{2+}	12.00	1.643 (-0.176)	1.454 (+0.038)
	Ca^{2+}	7.44	1.695 (-0.124)	1.445 (+0.029)
	Li^{+}	2.60	1.739 (-0.080)	1.434 (+0.018)
	Na^{+}	2.22	1.741 (-0.078)	1.432 (+0.016)
	K^{+}	1.47	1.757 (-0.062)	1.428 (+0.012)
	NH_4^{+}	1.64 (0.61)	1.754 (-0.065)	1.429 (+0.013)
Bis(benzene)tungsten	Without	0.00	1.831	1.418
	Mg^{2+}	11.78	1.660 (-0.171)	1.454 (+0.036)
	Ca^{2+}	7.65	1.711 (-0.120)	1.447 (+0.029)
	Li^{+}	2.58	1.754 (-0.077)	1.435 (+0.017)
	Na^{+}	2.25	1.755 (-0.076)	1.434 (+0.016)
	K^{+}	1.47	1.771 (-0.060)	1.430 (+0.012)
	NH_4^{+}	1.67 (0.64)	1.768 (-0.063)	1.431 (+0.013)

Table S4. Cation-π distances ($d_{cat-\pi}$) and interaction and binding energies (E_{int} and E_{bind}, respectively) calculated at the B3LYP/def2-TZVP level (in kcal/mol) for cation-π interactions of ferrocene, ruthenocene and osmocene. For NH_4^+ the $d_{cat-\pi}$ is N-center distance.

System	Cation	$d_{cat-\pi}$ (Å)	E_{int} (kcal/mol)	E_{bind} (kcal/mol)
Ferrocene	Mg^{2+}	1.900	-152.98	-149.25
	Ca^{2+}	2.271	-108.77	-107.32
	Li^+	1.837	-47.44	-46.86
	Na^+	2.346	-30.21	-29.79
	K^+	2.821	-20.46	-20.20
	NH_4^+	2.947	-21.17	-20.47
Ruthenocene	Mg^{2+}	1.892	-153.01	-149.68
	Ca^{2+}	2.266	-109.03	-107.75
	Li^+	1.836	-46.24	-45.67
	Na^+	2.347	-29.19	-28.78
	K^+	2.822	-19.58	-19.32
	NH_4^+	2.952	-20.24	-19.56
Osmocene	Mg^{2+}	1.890	-155.62	-150.08
	Ca^{2+}	2.253	-109.85	-107.86
	Li^+	1.829	-46.22	-45.39
	Na^+	2.339	-29.14	-28.52
	K^+	2.815	-19.48	-19.12
	NH_4^+	2.948	-20.18	-19.38

Table S5. Deformation energies od Cp sandwich compounds (E_{def}), metal-π distances ($d_{M-\pi}$), average lengths of the carbon-carbon bonds in the Cp aromatic rings interacting with the cations (d_{C-C}) for ferrocene, ruthenocene and osmocene. Calculations were done at the B3LYP/def2-TZVP level. In the brackets are the deformation energies of ammonium ion, as well as the changes in $d_{M-\pi}$ and d_{C-C} distances.

System	Cation	E_{def} (kcal/mol)	$d_{M-\pi}$ (Å)	d_{C-C} (Å)
Ferrocene	Without	0.00	1.690	1.423
	Mg^{2+}	3.72	1.626 (-0.064)	1.460 (+0.037)
	Ca^{2+}	1.45	1.655 (-0.035)	1.446 (+0.023)
	Li^+	0.58	1.667 (-0.023)	1.437 (+0.014)
	Na^+	0.42	1.667 (-0.023)	1.435 (+0.012)
	K^+	0.26	1.674 (-0.016)	1.431 (+0.008)
	NH_4^+	0.30 (0.40)	1.674 (-0.016)	1.431 (+0.008)
Ruthenocene	Without	0.00	1.840	1.427
	Mg^{2+}	3.33	1.797 (-0.043)	1.464 (+0.037)
	Ca^{2+}	1.28	1.823 (-0.017)	1.450 (+0.023)
	Li^+	0.57	1.825 (-0.015)	1.442 (+0.015)
	Na^+	0.41	1.824 (-0.016)	1.439 (+0.012)
	K^+	0.25	1.830 (-0.010)	1.436 (+0.009)
	NH_4^+	0.30 (0.38)	1.830 (-0.010)	1.436 (+0.009)
Osmocene	Without	0.00	1.856	1.430
	Mg^{2+}	5.53	1.770 (-0.086)	1.476 (+0.046)
	Ca^{2+}	1.98	1.809 (-0.047)	1.458 (+0.028)
	Li^+	0.84	1.824 (-0.032)	1.448 (+0.018)
	Na^+	0.61	1.826 (-0.030)	1.444 (+0.014)
	K^+	0.36	1.834 (-0.022)	1.440 (+0.010)
	NH_4^+	0.42 (0.38)	1.834 (-0.022)	1.441 (+0.011)

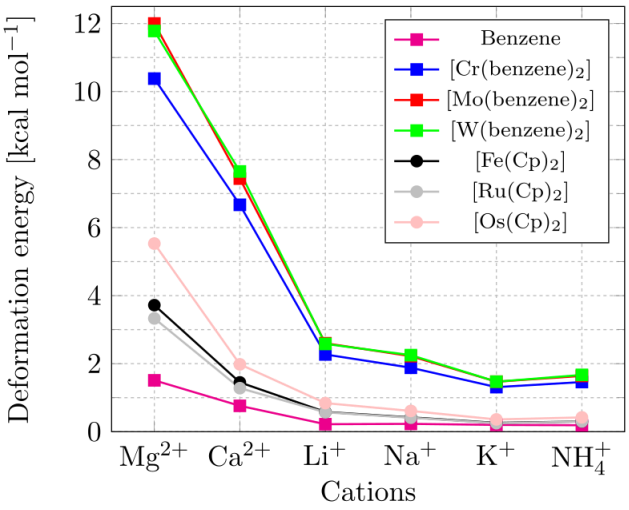


Figure S5. Deformation energies of benzene and Cp sandwich compounds (in kcal/mol) in interactions with various cations.

Table S6. The distance between the aromatic rings, $d_{\pi-\pi}$, the distance between the metal atom and the bottom aromatic ring, $d_{M-\pi,\ bottom}$, and the average length of the C-C bond in the bottom aromatic ring for benzene sandwich compounds. Calculations were done at the B3LYP/def2-TZVP level. The parameters are defined at Fig. S3. The values in brackets are the changes in the values of respective geometrical parameters due to the formation of cation-π interactions.

System	Cation	$d_{\pi-\pi}$ (Å)	$d_{M-\pi,\ bottom}$ (Å)	$d_{C-C,\ bottom}$ (Å)
Bis(benzene)chromium	Without	3.302	1.651	1.413
	Mg^{2+}	3.295 (-0.007)	1.802 (+0.151)	1.406 (-0.007)
	Ca^{2+}	3.341 (+0.039)	1.801 (+0.150)	1.406 (-0.007)
	Li^{+}	3.300 (-0.002)	1.721 (+0.070)	1.408 (-0.005)
	Na^{+}	3.294 (-0.008)	1.714 (+0.063)	1.408 (-0.005)
	K^{+}	3.298 (-0.004)	1.705 (+0.054)	1.409 (-0.004)
	NH_4^{+}	3.298 (-0.004)	1.708 (+0.057)	1.409 (-0.004)
Bis(benzene)molybdenum	Without	3.639	1.819	1.416
	Mg^{2+}	3.615 (-0.024)	1.973 (+0.154)	1.408 (-0.008)
	Ca^{2+}	3.666 (+0.027)	1.971 (+0.152)	1.408 (-0.008)
	Li^{+}	3.633 (-0.006)	1.894 (+0.075)	1.411 (-0.005)
	Na^{+}	3.628 (-0.011)	1.887 (+0.068)	1.411 (-0.005)
	K^{+}	3.634 (-0.005)	1.877 (+0.058)	1.412 (-0.004)
	NH_4^{+}	3.632 (-0.007)	1.878 (+0.059)	1.412 (-0.004)
Bis(benzene)tungsten	Without	3.661	1.831	1.418
	Mg^{2+}	3.626 (-0.035)	1.966 (+0.135)	1.410 (-0.008)
	Ca^{2+}	3.684 (+0.023)	1.973 (+0.142)	1.409 (-0.009)
	Li^{+}	3.653 (-0.008)	1.899 (+0.068)	1.412 (-0.006)
	Na^{+}	3.648 (-0.013)	1.893 (+0.062)	1.413 (-0.005)
	K^{+}	3.654 (-0.007)	1.883 (+0.052)	1.413 (-0.005)
	NH_4^{+}	3.653 (-0.008)	1.885 (+0.054)	1.413 (-0.005)

Table S7. The distance between the aromatic rings, $d_{\pi-\pi}$, the distance between the metal atom and the bottom aromatic ring, $d_{M-\pi,\ bottom}$, and the average length of the C-C bond in the bottom aromatic ring for Cp sandwich compounds. Calculations were done at the B3LYP/def2-TZVP level. The parameters are defined at Fig. S3. The values in brackets are the changes in the values of respective geometrical parameters due to the formation of cation-π interactions.

System	Cation	$d_{\pi-\pi}$ (Å)	$d_{M-\pi,\ bottom}$ (Å)	$d_{C-C,\ bottom}$ (Å)
Ferrocene	Without	3.380	1.690	1.423
	Mg^{2+}	3.334 (-0.046)	1.708 (+0.018)	1.421 (-0.002)
	Ca^{2+}	3.362 (-0.018)	1.707 (+0.017)	1.421 (-0.002)
	Li^{+}	3.363 (-0.017)	1.696 (+0.006)	1.421 (-0.002)
	Na^{+}	3.363 (-0.017)	1.696 (+0.006)	1.422 (-0.001)
	K^{+}	3.369 (-0.011)	1.695 (+0.005)	1.422 (-0.001)
	NH_4^{+}	3.369 (-0.011)	1.694 (+0.004)	1.422 (-0.001)
Ruthenocene	Without	3.680	1.840	1.427
	Mg^{2+}	3.645 (-0.035)	1.848 (+0.008)	1.425 (-0.002)
	Ca^{2+}	3.667 (-0.013)	1.844 (+0.004)	1.425 (-0.002)
	Li^{+}	3.662 (-0.018)	1.837 (-0.003)	1.425 (-0.002)
	Na^{+}	3.663 (-0.017)	1.839 (-0.001)	1.425 (-0.002)
	K^{+}	3.669 (-0.011)	1.839 (-0.001)	1.426 (-0.001)
	NH_4^{+}	3.669 (-0.011)	1.839 (-0.001)	1.426 (-0.001)
Osmocene	Without	3.712	1.856	1.430
	Mg^{2+}	3.653 (-0.059)	1.883 (+0.027)	1.427 (-0.003)
	Ca^{2+}	3.684 (-0.028)	1.875 (+0.019)	1.427 (-0.003)
	Li^{+}	3.687 (-0.025)	1.863 (+0.007)	1.428 (-0.002)
	Na^{+}	3.690 (-0.022)	1.864 (+0.008)	1.428 (-0.002)
	K^{+}	3.696 (-0.016)	1.862 (+0.006)	1.428 (-0.002)
	NH_4^{+}	3.696 (-0.016)	1.862 (+0.006)	1.428 (-0.002)

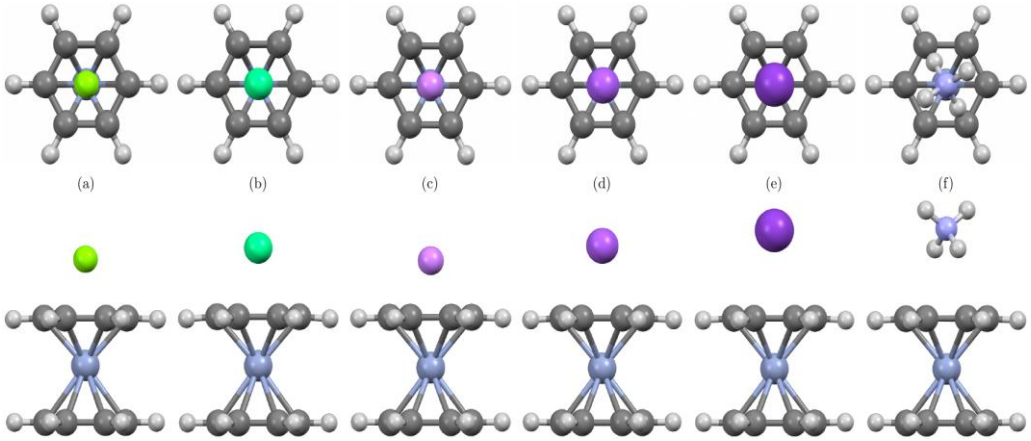


Figure S6. Cation-π interactions between bis(benzene)chromium and cations: (a) Mg^{2+}, (b) Ca^{2+}, (c) Li^{+}, (d) Na^{+}, (e) K^{+} and (f) NH_4^{+}. Calculations were done at the B3LYP/def2-TZVP level.

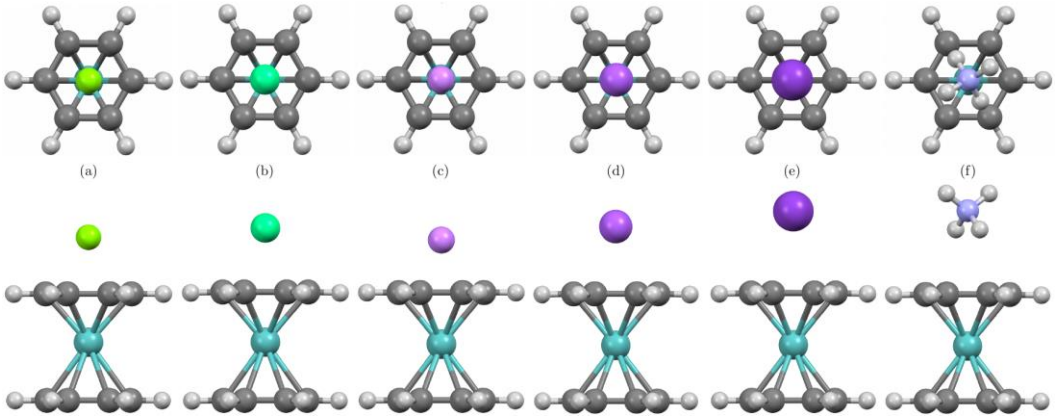


Figure S7. Cation-π interactions between bis(benzene)molybdenum and cations: (a) Mg^{2+}, (b) Ca^{2+}, (c) Li^{+}, (d) Na^{+}, (e) K^{+} and (f) NH_4^{+}. Calculations were done at the B3LYP/def2-TZVP level.

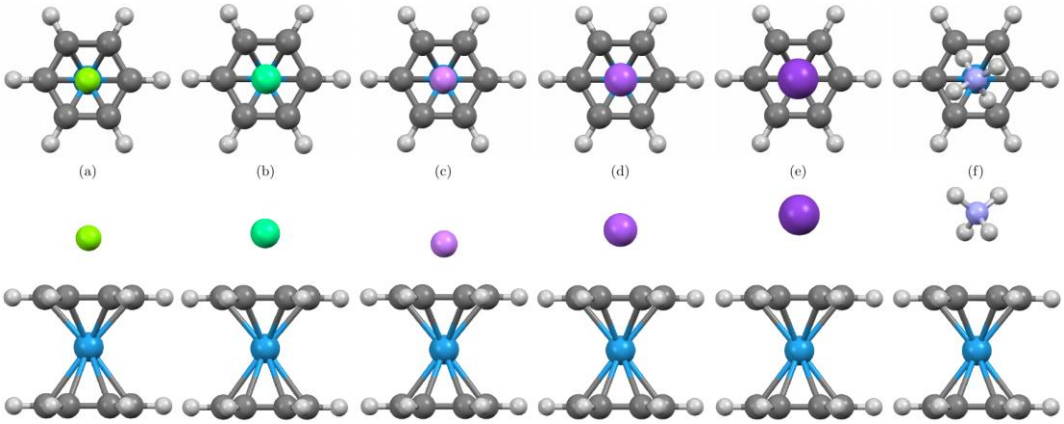


Figure S8. Cation-π interactions between bis(benzene)tungsten and cations: (a) Mg^{2+}, (b) Ca^{2+}, (c) Li^{+}, (d) Na^{+}, (e) K^{+} and (f) NH_4^{+}. Calculations were done at the B3LYP/def2-TZVP level.

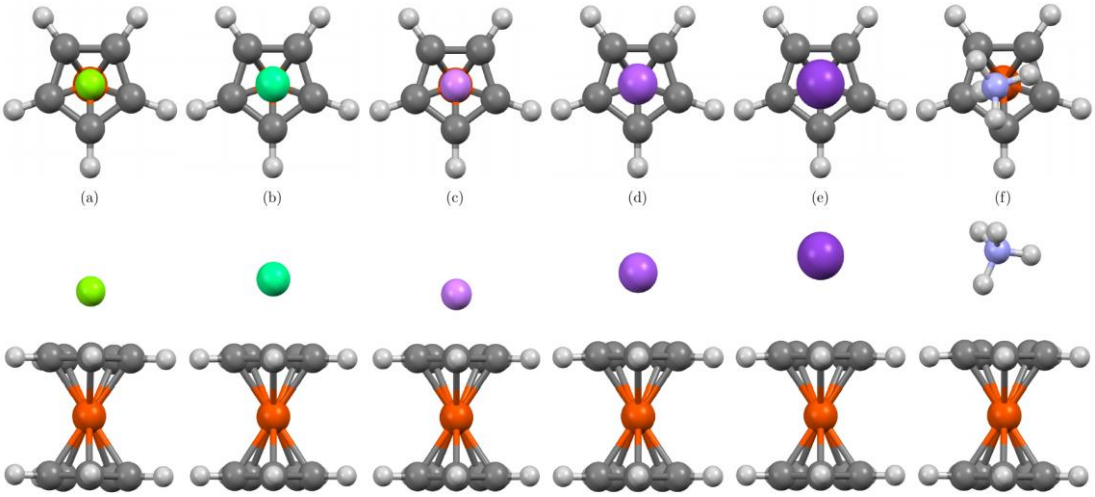


Figure S9. Cation-π interactions between ferrocene and cations: (a) Mg^{2+}, (b) Ca^{2+}, (c) Li^{+}, (d) Na^{+}, (e) K^{+} and (f) NH_4^{+}. Calculations were done at the B3LYP/def2-TZVP level.

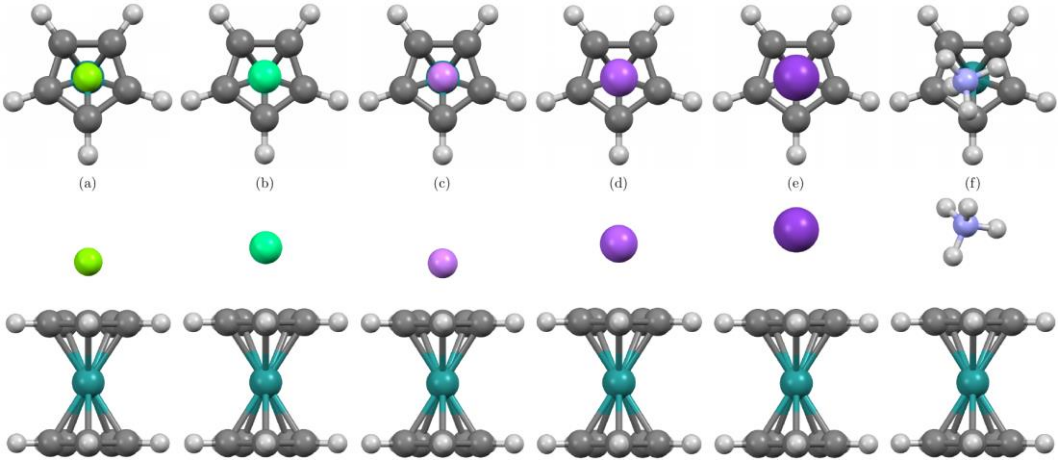


Figure S10. Cation-π interactions between ruthenocene and cations: (a) Mg^{2+}, (b) Ca^{2+}, (c) Li^{+}, (d) Na^{+}, (e) K^{+} and (f) NH_4^{+}. Calculations were done at the B3LYP/def2-TZVP level.

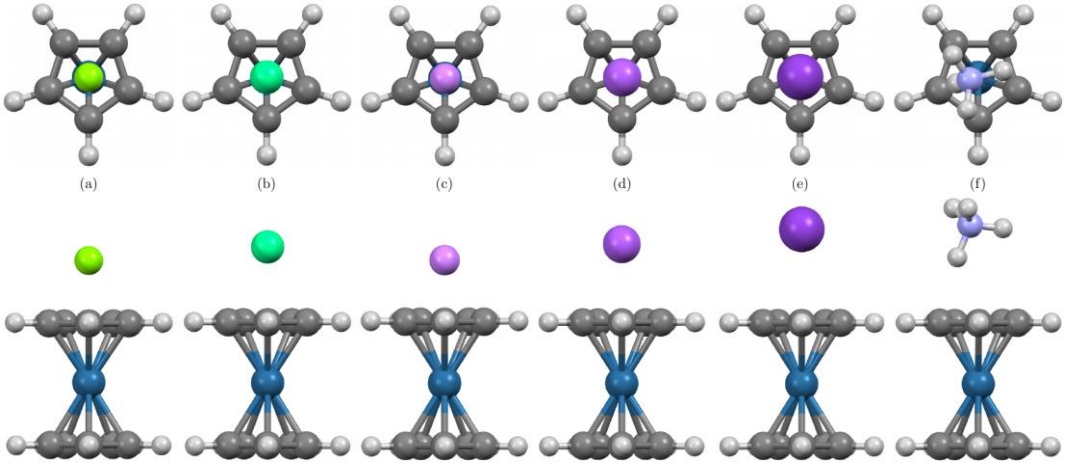


Figure S11. Cation-π interactions between osmocene and cations: (a) Mg^{2+}, (b) Ca^{2+}, (c) Li^{+}, (d) Na^{+}, (e) K^{+} and (f) NH_4^{+}. Calculations were done at the B3LYP/def2-TZVP level.

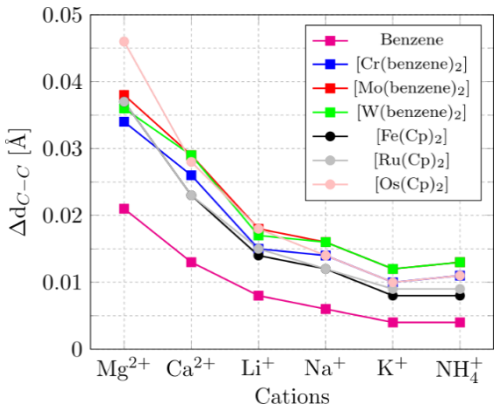


Figure S12. Changes in average lengths of carbon-carbon bonds in the interacting benzene ring, $\Delta d_{C\text{-}C}$ (Figure 1), for sandwich compounds due to interactions with various cations, calculated at the B3LYP/def2-TZVP level.

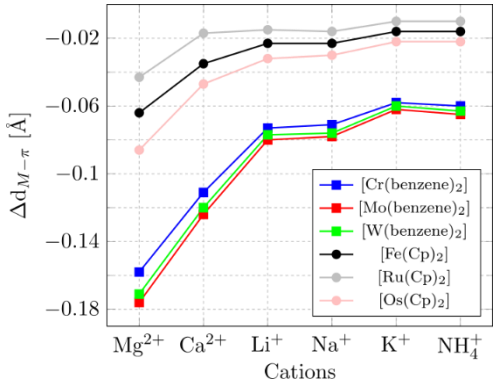


Figure S13. The changes in distances between metal atom and aromatic ring, $\Delta d_{M\text{-}\pi}$ (Figure 1), for sandwich compounds due to interactions with various cations, calculated at the B3LYP/def2-TZVP level.

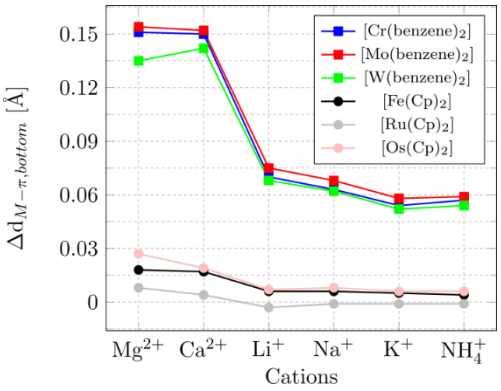


Figure S14. The changes in distance between metal atom and bottom (non-interacting) aromatic ring, $\Delta d_{M\text{-}\pi,bottom}$ (Figure 1), for sandwich compounds due to interactions with various cations, calculated at the B3LYP/def2-TZVP level.

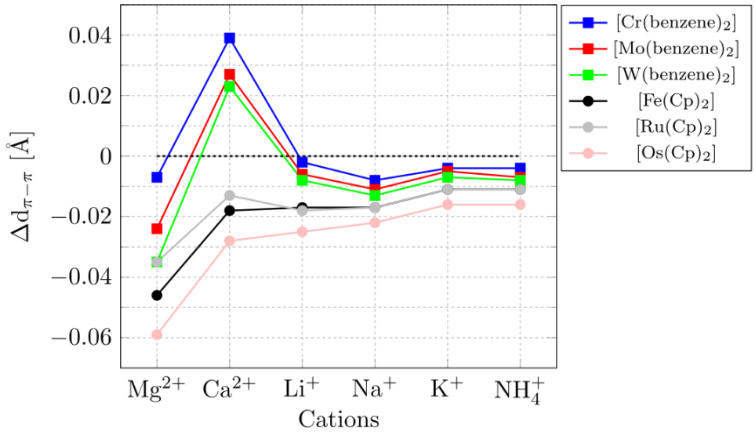


Figure S15. The changes in distances between aromatic rings in sandwich compounds, $\Delta d_{\pi\text{-}\pi}$ (Figure 1), due to formation of cation-π interactions, calculated at the B3LYP/def2-TZVP level.

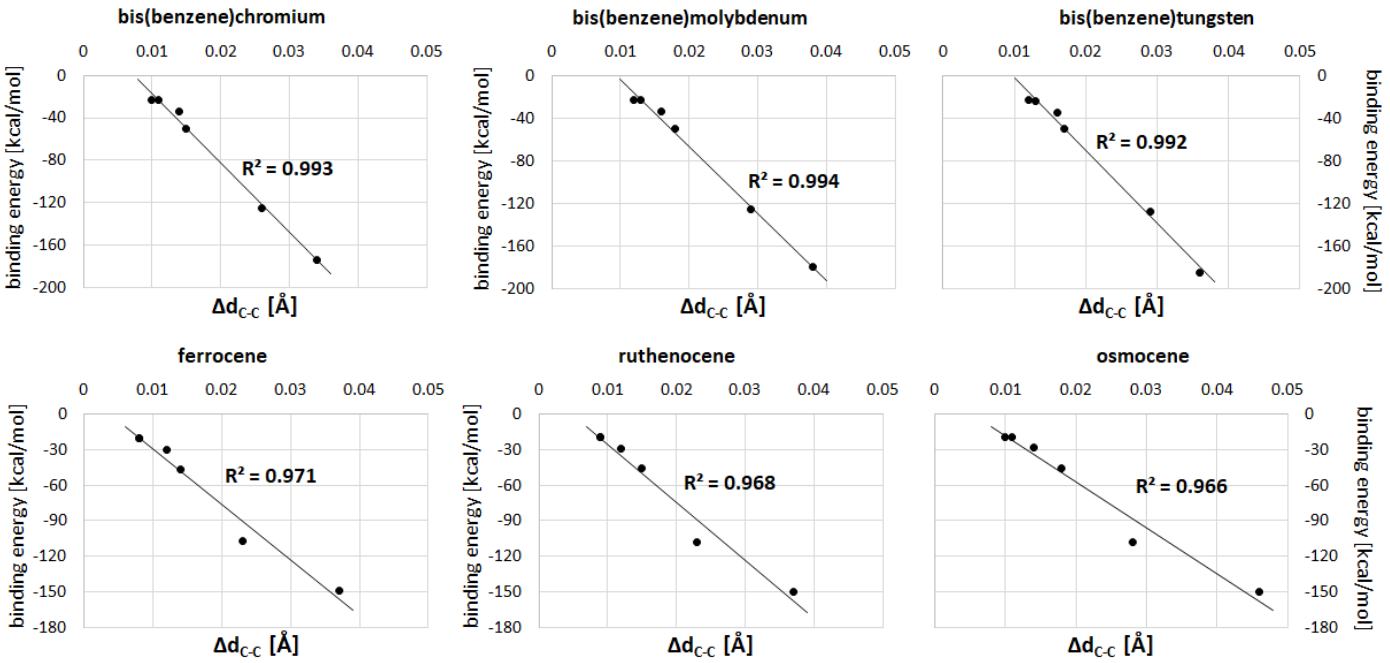


Figure S16. Correlation between changes in C-C bond lengths in interacting aromatic rings of sandwich compounds and cation-π binding energies, calculated at the B3LYP/def2-TZVP level.

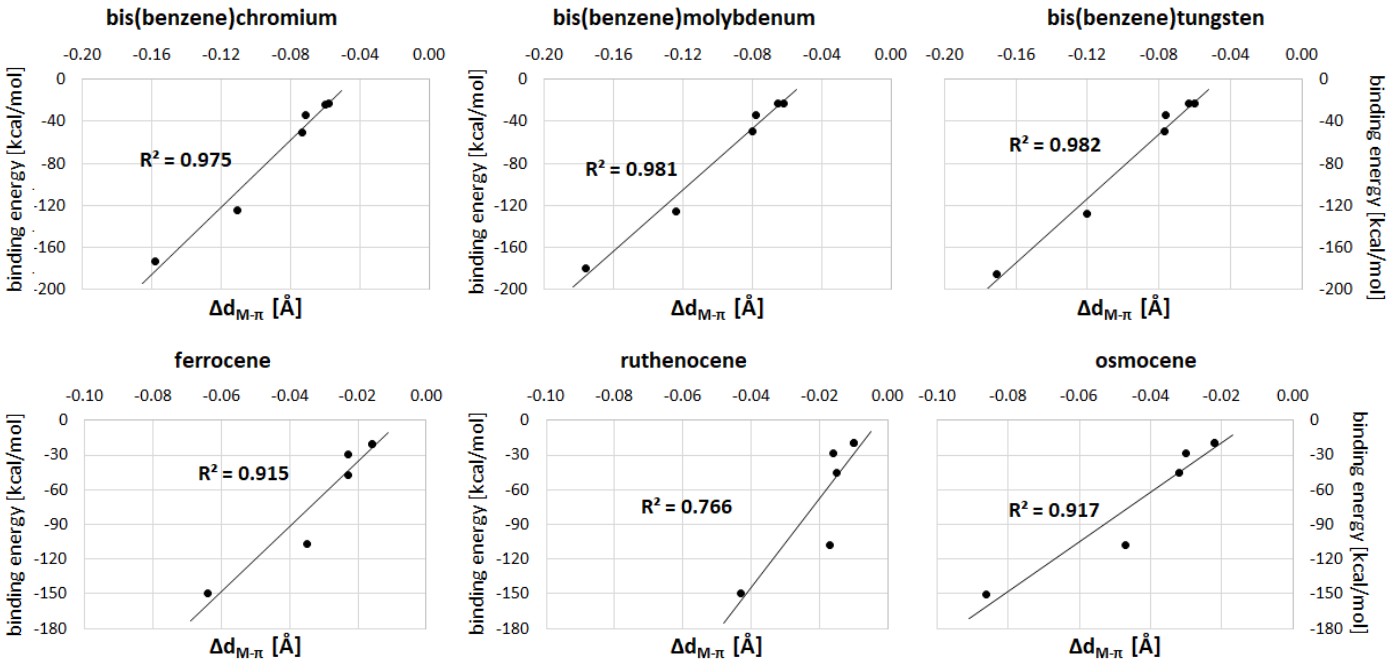
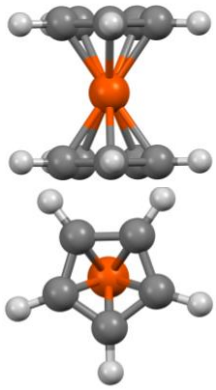


Figure S17. Correlation between changes in M-π distances in interacting sandwich compounds and cation-π binding energies, calculated at B3LYP/def2-TZVP level.

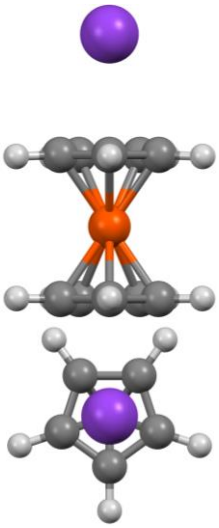
Coordinates for ferrocene and cation-ferrocene complexes

Ferrocene



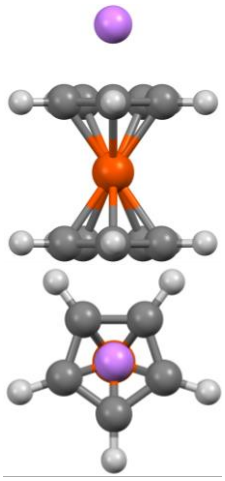
C	0.011680	-0.335785	0.015966
C	-0.024435	-0.346975	1.438457
C	1.375744	-0.329672	-0.389240
C	2.182690	-0.336930	0.782869
C	1.317307	-0.347718	1.912418
H	-0.843977	-0.349090	-0.639581
H	1.734740	-0.337002	-1.405675
H	3.260243	-0.350838	0.810121
H	1.624196	-0.371291	2.945539
H	-0.912211	-0.369830	2.049524
Fe	0.976398	-2.029293	0.738868
C	0.019310	-3.715743	-0.010151
C	-0.016587	-3.726833	1.412371
C	1.325217	-3.727340	1.886125
C	1.383283	-3.709333	-0.415552
C	2.190413	-3.716483	0.756448
H	1.742279	-3.684934	-1.431719
H	-0.836536	-3.696287	-0.665299
H	-0.904423	-3.717401	2.023697
H	1.632309	-3.718540	2.919418
H	3.267898	-3.698024	0.783621

K^+-Ferrocene



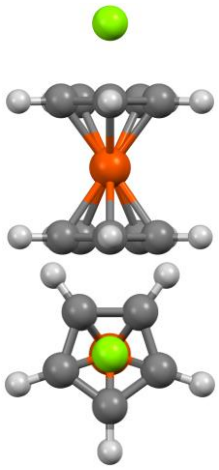
C	0.002258	-0.017270	0.001686
C	0.002253	-0.017284	1.433204
C	1.363703	-0.017278	1.875540
C	2.205100	-0.017300	0.717443
C	1.363690	-0.017340	-0.440655
Fe	0.987389	-1.690883	0.717435
C	0.009130	-3.386021	1.428440
C	1.361295	-3.386068	1.867440
C	2.196653	-3.386065	0.717143
C	1.360792	-3.385974	-0.432789
C	0.008833	-3.385993	0.006785
H	-0.863314	-3.374969	-0.626600
H	-0.862750	-3.375001	2.062206
H	1.694608	-3.375157	2.892498
H	3.274537	-3.375146	0.716933
H	1.693645	-3.374996	-1.458009
H	-0.869793	-0.054271	2.066812
H	-0.869781	-0.054344	-0.631901
H	1.696778	-0.054436	-1.465833
H	3.283012	-0.054311	0.717467
H	1.696798	-0.054273	2.900705
K	0.987252	2.804087	0.717254

Li^+-Ferrocene



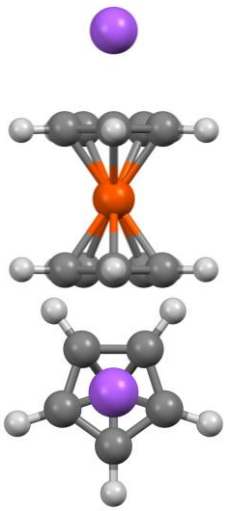
C	-0.009537	-0.024496	-0.009812
C	-0.009595	-0.023481	1.427671
C	1.357612	-0.023360	1.871905
C	2.202480	-0.024248	0.708863
C	1.357520	-0.024974	-0.454000
Fe	0.979371	-1.691528	0.710690
C	0.000937	-3.386640	1.422525
C	1.352826	-3.386651	1.861622
C	2.188156	-3.387496	0.711570
C	1.352543	-3.388052	-0.438278
C	0.000767	-3.387502	0.001128
H	3.266118	-3.375129	0.711428
H	1.685517	-3.376124	-1.463526
H	-0.871392	-3.375191	-0.632390
H	-0.871092	-3.373631	2.056224
H	1.686060	-3.373621	2.886773
H	1.690558	-0.037476	-1.479123
H	3.280362	-0.035911	0.708853
H	1.690722	-0.033905	2.897034
H	-0.881628	-0.034161	2.061259
H	-0.881565	-0.036377	-0.643362
Li	0.979690	1.812743	0.709888

Mg^{2+}-Ferrocene



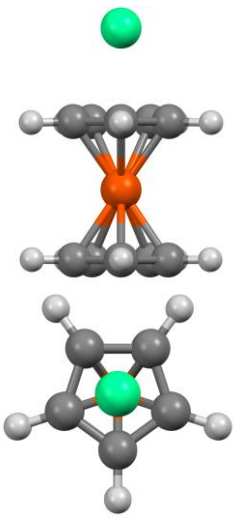
C	0.000244	0.055407	0.000845
C	0.000490	0.055556	1.422239
C	1.352376	0.055562	1.861203
C	2.187642	0.055367	0.711153
C	1.351963	0.055284	-0.438625
Fe	0.978555	1.763499	0.711102
C	1.362495	3.388655	-0.470843
C	-0.026499	3.388559	-0.020145
C	-0.026999	3.389177	1.439994
C	1.361512	3.390492	1.891757
C	2.220219	3.389486	0.710779
H	-0.872663	0.060875	-0.633117
H	-0.872141	0.061141	2.056563
H	1.685944	0.061032	2.887164
H	3.266462	0.060877	0.711036
H	1.685134	0.060718	-1.464715
H	-0.900559	3.372906	2.074255
H	-0.899674	3.370792	-0.654897
H	1.696634	3.371314	-1.497342
H	3.299759	3.373502	0.711243
H	1.694732	3.373282	2.918558
Mg	0.977561	5.288997	0.708966

Na^+-Ferrocene



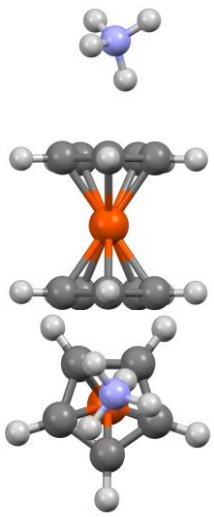
C	-0.000108	-0.017850	-0.000166
C	-0.000035	-0.017813	1.421417
C	1.351982	-0.017730	1.860610
C	2.187490	-0.017750	0.710508
C	1.351865	-0.017821	-0.439508
Fe	0.978185	1.677839	0.710556
C	1.355430	3.344599	-0.450370
C	-0.009249	3.344612	-0.007199
C	-0.009469	3.344762	1.427645
C	1.355064	3.344859	1.871217
C	2.198612	3.344725	0.710553
H	3.265396	-0.006497	0.710409
H	1.684914	-0.006617	-1.464673
H	-0.872163	-0.006620	-0.633728
H	-0.872036	-0.006564	2.055047
H	1.685123	-0.006468	2.885753
H	1.688676	3.312302	-1.475459
H	3.276506	3.312584	0.710686
H	1.687984	3.312831	2.896429
H	-0.881591	3.312604	2.061095
H	-0.881169	3.312315	-0.640927
Na	0.978191	5.690579	0.709898

Ca^{2+}-Ferrocene



C	0.009577	-0.001136	0.006985
C	0.009678	-0.001146	1.453168
C	1.385110	-0.001158	1.900004
C	2.235109	-0.001228	0.729956
C	1.384980	-0.001180	-0.439989
Fe	1.004874	-1.656410	0.730168
C	0.027309	-3.362944	1.441885
C	1.379049	-3.362765	1.880169
C	2.213634	-3.363270	0.730065
C	1.377668	-3.363625	-0.419069
C	0.026426	-3.363439	0.020864
H	1.712983	-3.355447	2.905839
H	3.292263	-3.356311	0.729431
H	1.710349	-3.357046	-1.445117
H	-0.846604	-3.356583	-0.612592
H	-0.844942	-3.355719	2.076424
H	3.314932	-0.026119	0.729881
H	1.718848	-0.025914	2.926996
H	-0.863896	-0.025923	2.087909
H	-0.864075	-0.025973	-0.627665
H	1.718580	-0.025995	-1.466995
Ca	1.004911	2.269873	0.729978

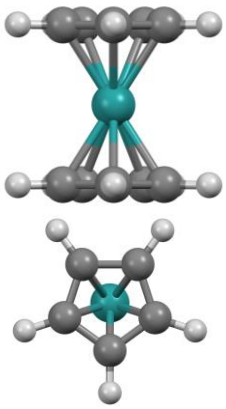
NH_4^+-Ferrocene



C	-0.045730	0.028846	-0.005904
C	-0.028217	0.005074	1.415386
C	1.328835	-0.040174	1.836953
C	2.149678	-0.044338	0.676112
C	1.300023	-0.001663	-0.463021
Fe	0.990159	1.683002	0.720649
C	1.409358	3.360677	-0.410085
C	0.048699	3.398348	0.048771
C	0.069502	3.367470	1.484731
C	1.434171	3.329201	1.903815
C	2.259223	3.325018	0.737031
H	3.227353	-0.062642	0.662469
H	1.620311	0.016886	-1.492089
H	-0.925004	0.075473	-0.627815
H	-0.891599	0.029627	2.060271
H	1.675138	-0.054769	2.857623
H	1.728583	3.339883	-1.439839
H	3.335802	3.265327	0.723573
H	1.780133	3.273213	2.923590
H	-0.795022	3.352677	2.129022
H	-0.832112	3.384649	-0.574016
N	0.918229	6.299155	0.653278
H	1.183116	6.818972	-0.184323
H	0.218705	6.823849	1.179883
H	0.544394	5.354214	0.392378
H	1.742050	6.137160	1.236249

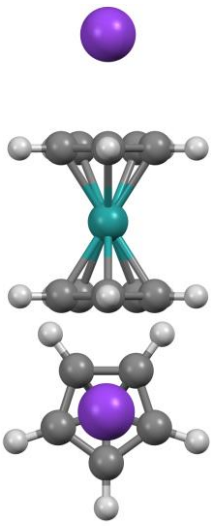
Coordinates for ruthenocene and cation-ruthenocene complexes

Ruthenocene



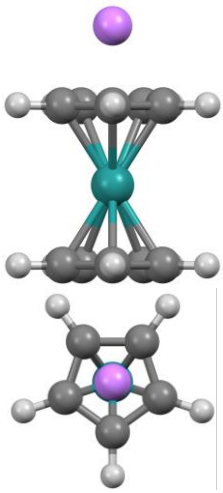
C	-0.002610	0.150162	-0.001914
C	-0.002612	0.150232	1.424877
C	1.354364	0.150231	1.865803
C	2.193003	0.150335	0.711501
C	1.354366	0.150387	-0.442778
Ru	0.979342	-1.689867	0.711358
C	-0.002718	-3.529953	1.424774
C	1.354320	-3.530163	1.865507
C	2.192798	-3.530209	0.711087
C	1.353998	-3.530014	-0.443073
C	-0.002915	-3.529698	-0.002018
H	3.270548	-3.543988	0.710847
H	1.686938	-3.543656	-1.468094
H	-0.874920	-3.542953	-0.635417
H	-0.874564	-3.543479	2.058365
H	1.687559	-3.543924	2.890453
H	1.687450	0.164130	-1.467750
H	3.270756	0.163994	0.711412
H	1.687460	0.163817	2.890797
H	-0.874546	0.163774	2.058347
H	-0.874524	0.163596	-0.635434

K^+-Ruthenocene



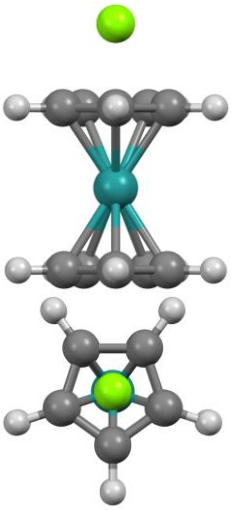
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.435506
C	1.365258	0.000000	1.879105
C	2.209023	-0.000167	0.717804
C	1.365267	-0.000055	-0.443569
Ru	0.987666	-1.830082	0.717882
C	0.006241	-3.668387	1.431376
C	1.362117	-3.668666	1.871791
C	2.199963	-3.669240	0.718418
C	1.361903	-3.669551	-0.434855
C	0.006109	-3.669028	0.005778
H	-0.865835	-3.682126	-0.627528
H	-0.865558	-3.680915	2.064896
H	1.695236	-3.681428	2.896668
H	3.277618	-3.682617	0.718323
H	1.694911	-3.683145	-1.459766
H	-0.872607	-0.009662	2.069473
H	-0.872620	-0.009668	-0.633951
H	1.698694	-0.009763	-1.469324
H	3.287614	-0.009988	0.717852
H	1.698570	-0.009772	2.904892
K	0.988368	2.821859	0.717784

Li^+-Ruthenocene



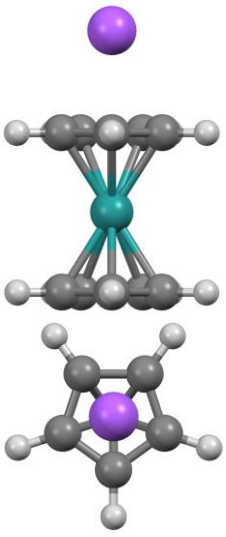
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.441988
C	1.371439	0.000000	1.887543
C	2.218995	0.000072	0.720897
C	1.371389	-0.000027	-0.445646
Ru	0.992245	-1.824497	0.720853
C	0.011273	-3.661652	1.433691
C	1.366980	-3.661801	1.873918
C	2.204578	-3.661853	0.720587
C	1.366572	-3.661642	-0.432393
C	0.011058	-3.661554	0.008309
H	-0.860978	-3.671807	-0.625049
H	-0.860600	-3.671870	2.067268
H	1.700270	-3.672318	2.898870
H	3.282358	-3.672371	0.720376
H	1.699353	-3.671835	-1.457514
H	-0.872107	0.013959	2.075565
H	-0.872069	0.014478	-0.633635
H	1.704369	0.013944	-1.470903
H	3.296959	0.013451	0.720841
H	1.704585	0.013409	2.912746
Li	0.991167	1.835527	0.720187

Mg^{2+}-Ruthenocene



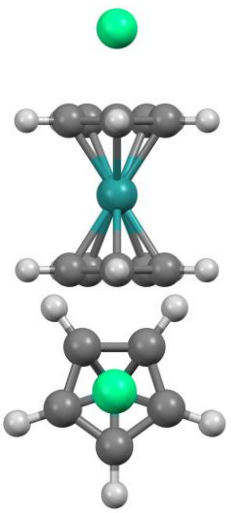
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.464359
C	1.392736	0.000000	1.916859
C	2.253472	0.000073	0.732071
C	1.392660	0.000045	-0.452561
Ru	1.007930	-1.797083	0.732205
C	0.027576	-3.644986	1.445104
C	1.382987	-3.644637	1.885270
C	2.220441	-3.644600	0.732193
C	1.382632	-3.644760	-0.420616
C	0.027363	-3.645086	0.019972
H	-0.845290	-3.656738	-0.613927
H	-0.844927	-3.656549	2.079217
H	1.716501	-3.655859	2.911008
H	3.299021	-3.655804	0.732019
H	1.715789	-3.656108	-1.446463
H	-0.873628	0.006452	2.099103
H	-0.873603	0.006667	-0.634788
H	1.726366	0.006557	-1.479589
H	3.333340	0.006247	0.731980
H	1.726517	0.006118	2.943850
Mg	1.007302	1.892344	0.731867

Na^+-Ruthenocene



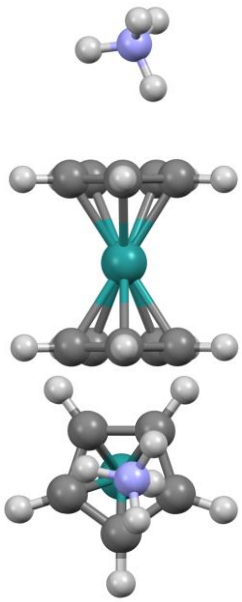
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.438985
C	1.368492	0.000000	1.883582
C	2.214255	0.000000	0.719574
C	1.368597	0.000048	-0.444589
Ru	0.989910	-1.824421	0.719173
C	0.008791	-3.663462	1.431859
C	1.364553	-3.663495	1.872275
C	2.202353	-3.663437	0.718984
C	1.364394	-3.663393	-0.434208
C	0.008678	-3.663281	0.006336
H	-0.863200	-3.675186	-0.627112
H	-0.863032	-3.675665	2.065369
H	1.697638	-3.675590	2.897212
H	3.280050	-3.675619	0.718901
H	1.697358	-3.675459	-1.459171
H	-0.872500	-0.005053	2.072886
H	-0.872470	-0.004957	-0.633972
H	1.701886	-0.004979	-1.470264
H	3.292714	-0.005253	0.719632
H	1.701723	-0.005410	2.909268
Na	0.985996	2.347165	0.716387

Ca^{2+}-Ruthenocene



C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.449848
C	1.378865	0.000000	1.897868
C	2.231050	-0.000024	0.724936
C	1.378894	0.000009	-0.447999
Ru	0.997561	-1.822615	0.724728
C	0.017199	-3.667308	1.437065
C	1.372436	-3.667116	1.877325
C	2.209943	-3.666846	0.724461
C	1.372296	-3.666919	-0.428283
C	0.017120	-3.667139	0.012123
H	-0.855378	-3.678128	-0.621685
H	-0.855195	-3.678371	2.071014
H	1.705702	-3.678099	2.902942
H	3.288351	-3.677514	0.724398
H	1.705483	-3.677712	-1.453922
H	-0.873990	-0.001602	2.084880
H	-0.874016	-0.001150	-0.635013
H	1.712755	-0.001534	-1.475450
H	3.311374	-0.002329	0.724935
H	1.712679	-0.002249	2.925323
Ca	0.996642	2.265810	0.724116

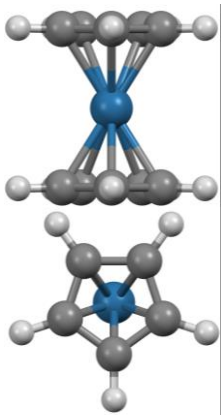
NH_4^+-Ruthenocene



C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.432500
C	1.361218	0.000000	1.879519
C	2.210970	-0.001211	0.726734
C	1.371236	0.010204	-0.442869
Ru	0.991967	-1.828192	0.703016
C	0.009543	-3.668029	1.405288
C	1.364890	-3.669601	1.848860
C	2.205297	-3.667586	0.697352
C	1.369500	-3.663823	-0.457340
C	0.012680	-3.664788	-0.020202
H	-0.857667	-3.676086	-0.655694
H	-0.863526	-3.682408	2.036987
H	1.695471	-3.685464	2.874516
H	3.282920	-3.681369	0.699467
H	1.704668	-3.673233	-1.481659
H	-0.873970	-0.005676	2.064092
H	-0.870264	0.000599	-0.636837
H	1.708069	-0.005695	-1.467749
H	3.289292	-0.000335	0.730870
H	1.689966	-0.007273	2.906544
N	1.048546	2.943438	0.480237
H	0.827828	2.819663	1.470608
H	1.926500	3.455076	0.382417
H	1.140024	1.983253	0.068481
H	0.295750	3.456008	0.019031

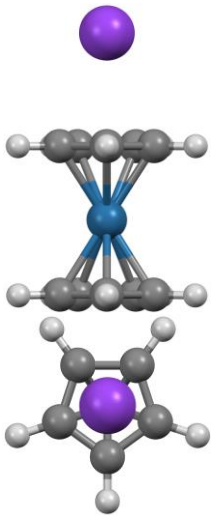
Coordinates for osmocene and cation-osmocene complexes

Osmocene



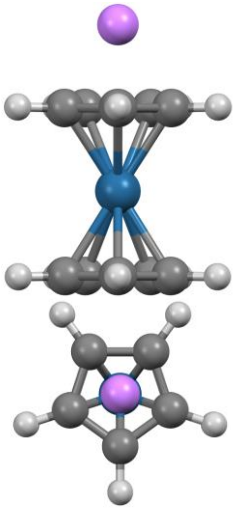
C	-0.004882	0.165914	-0.003561
C	-0.004846	0.165807	1.426500
C	1.355251	0.165757	1.868429
C	2.195836	0.165979	0.711494
C	1.355237	0.166118	-0.445474
Os	0.979388	-1.689867	0.711342
C	-0.004956	-3.545528	1.426391
C	1.355201	-3.545688	1.868133
C	2.195629	-3.545853	0.711084
C	1.354872	-3.545747	-0.445769
C	-0.005187	-3.545448	-0.003670
H	3.272995	-3.567278	0.711029
H	1.687603	-3.567093	-1.470464
H	-0.876931	-3.566530	-0.636761
H	-0.876473	-3.566676	2.059735
H	1.688257	-3.566849	2.892721
H	1.688112	0.187568	-1.470120
H	3.273205	0.187284	0.711587
H	1.688169	0.186741	2.893065
H	-0.876447	0.186971	2.059728
H	-0.876538	0.187174	-0.636768

K^+-Osmocene



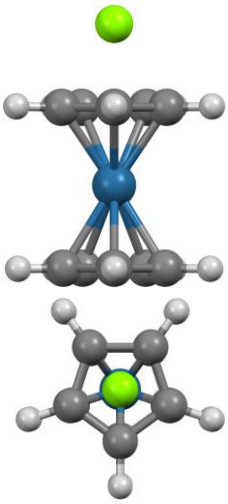
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.428264
C	1.358324	0.000000	1.869636
C	2.197834	0.000308	0.714108
C	1.358313	0.000214	-0.441394
Os	0.983009	-1.861891	0.713965
C	-0.007722	-3.695994	1.434145
C	1.362248	-3.696338	1.878971
C	2.208617	-3.696648	0.713551
C	1.361914	-3.696231	-0.451558
C	-0.007896	-3.695903	-0.006335
H	-0.880436	-3.694767	-0.640121
H	-0.880069	-3.695225	2.068187
H	1.695685	-3.695341	2.904545
H	3.287009	-3.695344	0.713465
H	1.695007	-3.694911	-1.477232
H	-0.871541	0.019788	2.061473
H	-0.871575	0.019718	-0.633197
H	1.691126	0.020273	-1.465991
H	3.275123	0.020508	0.714172
H	1.691194	0.019879	2.894213
K	0.970786	-6.511090	0.716848

Li^+-Osmocene



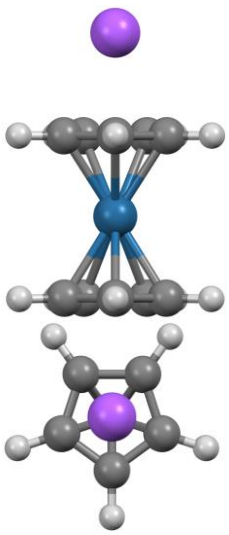
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.427796
C	1.357916	0.000000	1.869036
C	2.197179	0.000166	0.713932
C	1.357959	0.000174	-0.441198
Os	0.982850	-1.863010	0.714004
C	-0.013072	-3.687049	1.438311
C	1.363818	-3.686668	1.885671
C	2.214770	-3.687067	0.714448
C	1.363852	-3.687550	-0.456794
C	-0.013074	-3.687546	-0.009464
H	-0.884912	-3.709889	-0.642899
H	-0.884891	-3.709125	2.071780
H	1.696843	-3.707923	2.910601
H	3.292421	-3.708473	0.714475
H	1.696902	-3.709563	-1.481690
H	-0.871676	0.016649	2.061086
H	-0.871677	0.016561	-0.633299
H	1.690935	0.016993	-1.465887
H	3.274602	0.016990	0.713926
H	1.690853	0.016450	2.893751
Li	0.981991	-5.516004	0.715516

Mg^{2+}-Osmocene



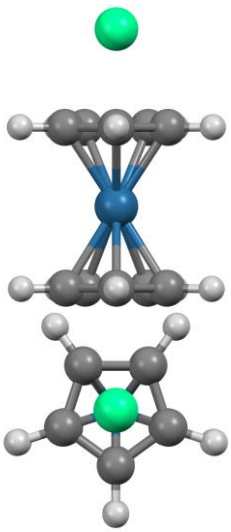
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.426747
C	1.356907	0.000000	1.867659
C	2.195530	0.000095	0.713351
C	1.356893	-0.000036	-0.440934
Os	0.981939	-1.882511	0.713386
C	-0.033382	-3.652706	1.451508
C	1.370490	-3.652613	1.907367
C	2.237804	-3.652578	0.713148
C	1.370154	-3.652651	-0.480825
C	-0.033572	-3.652607	-0.024575
H	-0.906853	-3.672624	-0.658870
H	-0.906503	-3.672930	2.086016
H	1.704175	-3.672436	2.933821
H	3.317130	-3.672008	0.713028
H	1.703533	-3.672263	-1.507372
H	-0.872402	0.015038	2.060575
H	-0.872433	0.014882	-0.633803
H	1.690078	0.014981	-1.466531
H	3.273877	0.015224	0.713319
H	1.690111	0.015043	2.893240
Mg	0.981286	-5.542926	0.713587

Na^+-Osmocene



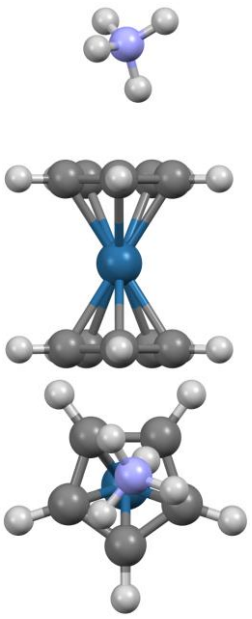
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.428017
C	1.358070	0.000000	1.869333
C	2.197478	0.000166	0.714030
C	1.358102	0.000340	-0.441271
Os	0.982736	-1.863548	0.713772
C	-0.010951	-3.689996	1.435470
C	1.362783	-3.690326	1.881620
C	2.211597	-3.690073	0.713000
C	1.362547	-3.689681	-0.455376
C	-0.011090	-3.689453	-0.008957
H	-0.883511	-3.692605	-0.642648
H	-0.883219	-3.693761	2.069333
H	1.696010	-3.694092	2.907101
H	3.289849	-3.693465	0.712927
H	1.695586	-3.692683	-1.480904
H	-0.871574	0.018449	2.061247
H	-0.871630	0.018450	-0.633199
H	1.690947	0.019066	-1.465896
H	3.274819	0.018920	0.714099
H	1.690889	0.018497	2.893979
Na	0.977719	-6.029388	0.713738

Ca^{2+}-Osmocene



C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.426994
C	1.357178	0.000000	1.867889
C	2.195904	-0.000237	0.713440
C	1.357146	-0.000241	-0.440968
Os	0.981913	-1.875075	0.713620
C	-0.020857	-3.684044	1.442746
C	1.365537	-3.684360	1.892832
C	2.221978	-3.684620	0.713513
C	1.365139	-3.684682	-0.465469
C	-0.021064	-3.684363	-0.014925
H	-0.895051	-3.690579	-0.649704
H	-0.894656	-3.690270	2.077819
H	1.699517	-3.690070	2.920072
H	3.302147	-3.689915	0.713368
H	1.698770	-3.690320	-1.492816
H	-0.872213	0.016784	2.060717
H	-0.872196	0.016857	-0.633719
H	1.690268	0.016418	-1.466327
H	3.274028	0.016422	0.713471
H	1.690403	0.016898	2.893219
Ca	0.979204	-5.937201	0.714740

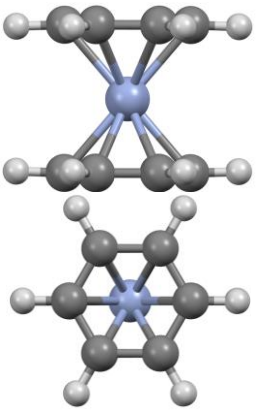
NH_4^+-Osmocene



C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.427960
C	1.357781	0.000000	1.870152
C	2.197891	-0.000925	0.715070
C	1.358467	-0.000998	-0.441103
Os	0.986147	-1.862218	0.712069
C	0.002866	-3.702135	1.426566
C	1.379215	-3.691926	1.870777
C	2.219308	-3.696692	0.704685
C	1.374113	-3.697831	-0.457824
C	0.005825	-3.693039	-0.018949
H	-0.866310	-3.703755	-0.652658
H	-0.869696	-3.692761	2.060723
H	1.712388	-3.700920	2.896111
H	3.297403	-3.700414	0.703323
H	1.708351	-3.701564	-1.482840
H	-0.871818	0.018486	2.060931
H	-0.871471	0.019622	-0.633289
H	1.691896	0.018880	-1.465477
H	3.275164	0.018951	0.715277
H	1.690015	0.019665	2.894915
N	0.789942	-6.632397	0.871248
H	0.481111	-5.661888	1.123502
H	1.084615	-7.137910	1.707794
H	1.579060	-6.536574	0.228898
H	0.029990	-7.136471	0.412380

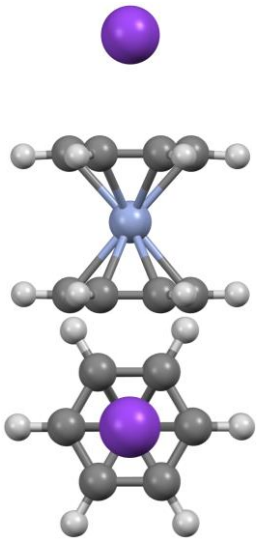
Coordinates for bis(benzene)chromium and cation-bis(benzene)chromium complexes

Bis(benzene)chromium



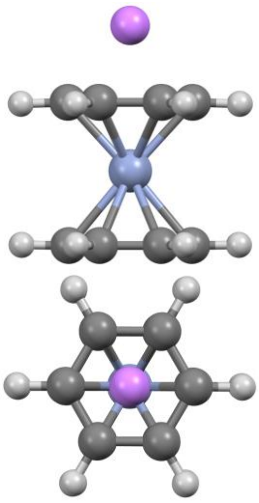
C	-0.022703	0.303318	-0.008261
C	-0.016744	0.306716	1.404376
C	1.197661	0.309414	-0.719746
C	2.423988	0.318691	-0.018627
C	1.209567	0.316113	2.105520
C	2.429916	0.322052	1.394023
H	3.368299	0.365156	1.930600
H	3.357866	0.358756	-0.563239
H	1.192962	0.343004	-1.801033
H	-0.961521	0.332586	-0.545003
H	-0.951043	0.337925	1.948851
H	1.213849	0.354495	3.186646
Cr	1.193219	1.963566	0.689004
C	2.409087	3.620562	-0.015885
C	2.403202	3.623716	1.396759
C	1.188697	3.611200	-0.727305
C	1.176906	3.617450	2.097955
C	-0.037605	3.605099	-0.026117
C	-0.043468	3.608189	1.386531
H	3.347922	3.588874	-0.552470
H	3.337492	3.594971	1.941376
H	1.172532	3.583992	3.179246
H	-0.981860	3.567445	1.923283
H	-0.971474	3.562467	-0.570541
H	1.193489	3.572647	-1.808428

K^+-Bis(benzene)chromium



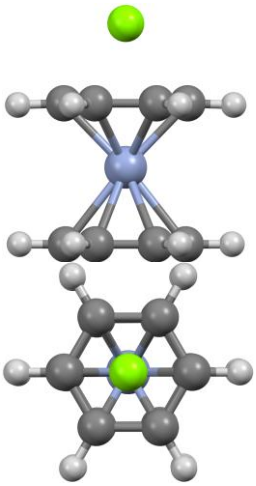
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.423382
C	1.232697	0.000000	2.135138
C	2.465445	0.000000	1.423382
C	2.465420	0.000043	-0.000062
C	1.232687	0.000043	-0.711753
Cr	1.232742	1.592716	0.711708
C	2.456971	3.298649	0.015520
C	1.241955	3.297659	-0.697717
C	0.016770	3.297260	-0.002131
C	0.006572	3.297702	1.406700
C	1.221575	3.298734	2.119958
C	2.446778	3.299282	1.424390
H	-0.935253	0.063394	1.963401
H	1.232748	0.063340	3.215105
H	3.400751	0.063400	1.963321
H	3.400658	0.063468	-0.540113
H	1.232612	0.063390	-1.791714
H	-0.935302	0.063381	-0.539928
H	1.213783	3.281995	3.201047
H	-0.933550	3.279991	1.940504
H	-0.915561	3.279194	-0.549420
H	1.249756	3.280045	-1.778792
H	3.397109	3.281713	-0.518281
H	3.379131	3.282866	1.971694
K	1.237769	-2.766644	0.714565

Li^+-Bis(benzene)chromium



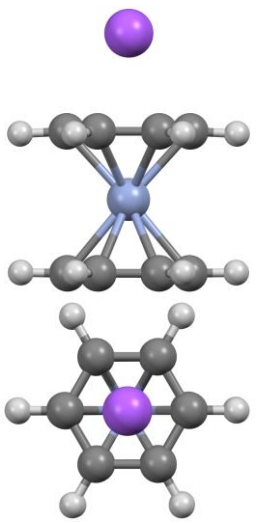
C	0.003379	0.027255	0.003294
C	0.004610	0.027430	1.411398
C	1.224672	0.027019	2.114424
C	2.443518	0.026435	1.409329
C	2.442290	0.026052	0.001219
C	1.222222	0.026461	-0.701806
Cr	1.222716	-1.694681	0.706627
C	1.232394	-3.272579	2.135509
C	2.464087	-3.273244	1.412046
C	2.453411	-3.273613	-0.016465
C	1.210867	-3.273191	-0.721309
C	-0.020729	-3.272334	0.002319
C	-0.009959	-3.272091	1.430665
H	1.240533	-3.238142	3.215566
H	3.403515	-3.239399	1.945078
H	3.384752	-3.240108	-0.563525
H	1.202771	-3.239251	-1.801389
H	-0.960113	-3.237760	-0.530731
H	-0.941252	-3.237363	1.977703
H	3.380208	0.011527	1.949102
H	1.225534	0.012598	3.195513
H	-0.931197	0.013396	1.952725
H	-0.933333	0.012965	-0.536456
H	1.221328	0.011615	-1.782890
H	3.378085	0.010979	-0.540103
Li	1.226992	-5.045481	0.703834

Mg^{2+}-Bis(benzene)chromium



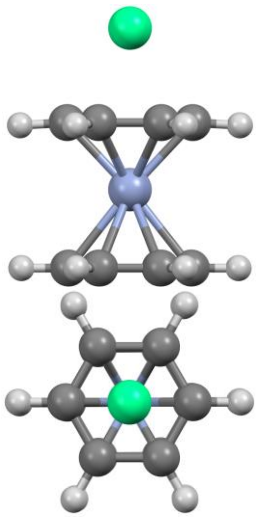
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.446888
C	1.253160	0.000000	2.170459
C	2.506457	-0.000066	1.446838
C	2.506280	-0.000175	-0.000361
C	1.252942	-0.000131	-0.723626
Cr	1.253554	1.492685	0.723509
C	2.475622	3.294418	0.028924
C	1.263194	3.294566	-0.682107
C	0.041230	3.294649	0.012359
C	0.031673	3.294649	1.417863
C	1.244088	3.294693	2.128915
C	2.466072	3.294546	1.434466
H	-0.934997	0.038281	1.986863
H	1.253332	0.038434	3.250183
H	3.441594	0.038387	1.986572
H	3.441295	0.038094	-0.540314
H	1.252851	0.038117	-1.803353
H	-0.935123	0.038306	-0.539756
H	1.236720	3.290491	3.210486
H	-0.908666	3.290463	1.952281
H	-0.891761	3.290381	-0.534789
H	1.270534	3.290233	-1.763677
H	3.415947	3.290087	-0.505520
H	3.399053	3.290264	1.981632
Mg	1.257350	-1.863766	0.725924

Na^+-Bis(benzene)chromium



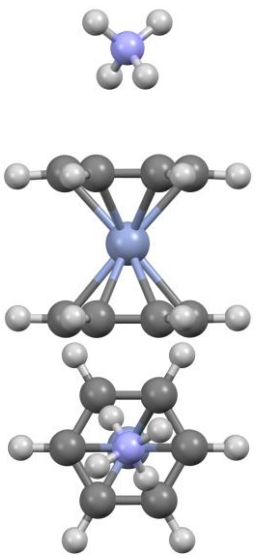
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.426369
C	1.235378	0.000000	2.139644
C	2.470887	-0.000065	1.426351
C	2.470737	-0.000367	-0.000279
C	1.235210	-0.000302	-0.713295
Cr	1.235905	1.580015	0.713188
C	2.459995	3.294151	0.016552
C	1.244904	3.293815	-0.695626
C	0.020577	3.293877	0.000565
C	0.011383	3.294190	1.408944
C	1.226475	3.294505	2.121123
C	2.450807	3.294527	1.424928
H	-0.935106	0.056878	1.966308
H	1.235336	0.057158	3.219439
H	3.406064	0.057129	1.966175
H	3.405804	0.056488	-0.540327
H	1.235107	0.056367	-1.793097
H	-0.935160	0.056747	-0.539823
H	1.219325	3.277945	3.202168
H	-0.928354	3.277439	1.943357
H	-0.912105	3.276788	-0.546042
H	1.252020	3.276677	-1.776662
H	3.399718	3.277417	-0.517888
H	3.383506	3.278019	1.971530
Na	1.249936	-2.276668	0.721837

Ca^{2+}-Bis(benzene)chromium



C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.438948
C	1.246206	0.000000	2.158474
C	2.492498	-0.000174	1.438956
C	2.492423	-0.000392	-0.000117
C	1.246143	-0.000239	-0.719512
Cr	1.246620	1.540127	0.719464
C	2.468938	3.340973	0.024844
C	1.256447	3.341328	-0.686208
C	0.034454	3.341512	0.008375
C	0.025009	3.341531	1.413934
C	1.237500	3.341410	2.124987
C	2.459496	3.341056	1.430402
H	-0.934974	0.062946	1.978796
H	1.246137	0.063084	3.238112
H	3.427520	0.062736	1.978739
H	3.427405	0.062359	-0.539990
H	1.246139	0.062578	-1.799156
H	-0.935009	0.062866	-0.539779
H	1.230157	3.342438	3.206548
H	-0.915324	3.342751	1.948356
H	-0.898586	3.342717	-0.538687
H	1.263754	3.342294	-1.767770
H	3.409261	3.341780	-0.509593
H	3.392537	3.341927	1.977464
Ca	1.248758	-2.170586	0.721226

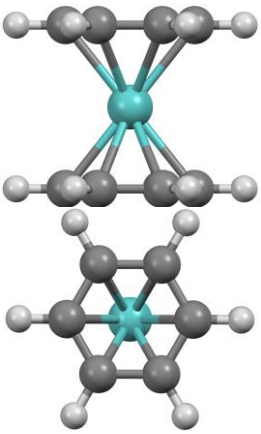
NH_4^+-Bis(benzene)chromium



C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.408523
C	1.220359	0.000000	2.111849
C	2.440500	-0.003642	1.406778
C	2.440497	-0.007284	-0.001740
C	1.220150	-0.003642	-0.705075
Cr	1.224057	1.705287	0.701178
C	2.459284	3.300788	-0.013012
C	1.224575	3.289669	-0.725568
C	-0.005507	3.293339	-0.014432
C	-0.004039	3.308096	1.411119
C	1.230623	3.293411	2.123709
C	2.460690	3.289784	1.412576
H	-0.936035	0.018112	1.949422
H	1.221201	0.019522	3.192906
H	3.376845	0.013111	1.947189
H	3.376608	0.005249	-0.542663
H	1.219504	0.013143	-1.786177
H	-0.936263	0.019554	-0.540457
H	1.228750	3.235815	3.203775
H	-0.938909	3.240514	1.951586
H	-0.942415	3.235557	-0.551767
H	1.226177	3.229445	-1.805493
H	3.393850	3.227760	-0.553291
H	3.397345	3.229401	1.950072
N	1.233208	6.133163	0.695635
H	0.527512	5.495438	1.103504
H	1.652962	6.715482	1.420464
H	1.937370	5.493076	0.289011
H	0.814811	6.715012	-0.030356

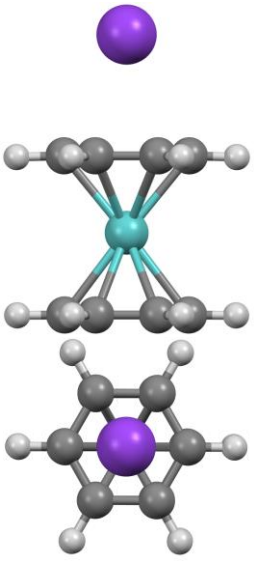
Coordinates for bis(benzene)molybdenum and cation-bis(benzene)molybdenum complexes

Bis(benzene)molybdenum



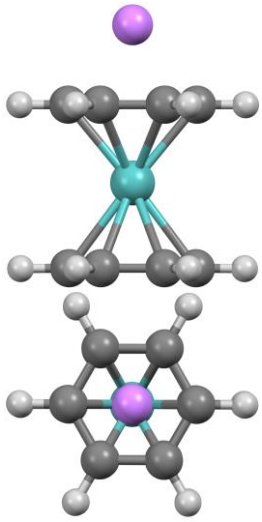
C	-0.003276	0.168399	-0.001126
C	-0.002556	0.168441	1.414975
C	1.224143	0.168378	2.122423
C	2.450138	0.168142	1.413776
C	2.449417	0.168183	-0.002324
C	1.222720	0.168378	-0.709772
Mo	1.223222	-1.650945	0.706333
C	1.234031	-3.470235	2.122431
C	2.454785	-3.470369	1.404795
C	2.443670	-3.470445	-0.011260
C	1.211808	-3.470312	-0.709675
C	-0.008946	-3.469973	0.007960
C	0.002168	-3.469973	1.424016
H	1.242540	-3.468707	3.204315
H	3.395976	-3.468924	1.938374
H	3.376349	-3.468996	-0.559594
H	1.203299	-3.468849	-1.791560
H	-0.950137	-3.468224	-0.525619
H	-0.930510	-3.468154	1.972350
H	3.387390	0.166447	1.954245
H	1.224708	0.166884	3.204340
H	-0.939231	0.166890	1.956451
H	-0.940528	0.166893	-0.541595
H	1.222154	0.166884	-1.791689
H	3.386092	0.166445	-0.543801

K^+-Bis(benzene)molybdenum



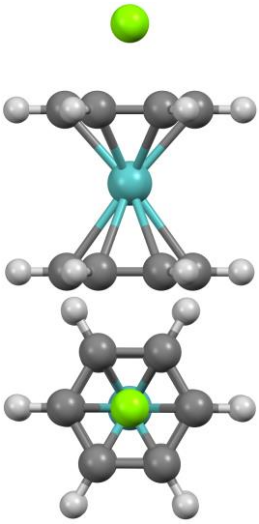
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.411873
C	1.222748	0.000000	2.117770
C	2.445452	-0.000256	1.411870
C	2.445452	-0.000704	-0.000002
C	1.222718	-0.000448	-0.705920
Mo	1.222325	-1.877383	0.706206
C	1.231255	-3.633902	2.134552
C	2.463298	-3.634093	1.412630
C	2.454166	-3.634262	-0.015313
C	1.212995	-3.634306	-0.721445
C	-0.019106	-3.633706	0.000483
C	-0.009948	-3.633472	1.428477
H	3.387465	-3.604901	-0.562172
H	1.206037	-3.605079	-1.803135
H	-0.959368	-3.604235	-0.534334
H	-0.943237	-3.603659	1.975348
H	1.238264	-3.604219	3.216226
H	3.403551	-3.604618	1.947433
H	1.222643	0.008077	-1.787145
H	3.381796	0.007757	-0.540682
H	3.381845	0.008486	1.952464
H	1.222841	0.008856	3.198993
H	-0.936338	0.009011	1.952554
H	-0.936433	0.008969	-0.540522
K	1.217969	-6.401070	0.704927

Li^+-Bis(benzene)molybdenum



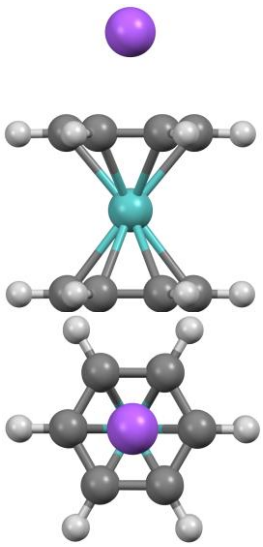
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.410924
C	1.221936	0.000000	2.116324
C	2.443795	-0.000363	1.410797
C	2.443795	-0.000768	-0.000127
C	1.221861	-0.000427	-0.705526
Mo	1.221475	-1.894315	0.705682
C	1.230129	-3.632962	2.139655
C	2.467234	-3.633360	1.415052
C	2.458387	-3.633491	-0.018598
C	1.212323	-3.633461	-0.727624
C	-0.024812	-3.633149	-0.003032
C	-0.015964	-3.632758	1.430639
H	3.391216	-3.630475	-0.564829
H	1.205575	-3.630553	-1.808597
H	-0.964264	-3.630006	-0.537807
H	-0.948793	-3.629239	1.976870
H	1.236892	-3.629644	3.220627
H	3.406695	-3.630311	1.949815
H	1.221869	0.009099	-1.786682
H	3.380131	0.008382	-0.540652
H	3.380071	0.009120	1.951438
H	1.221939	0.009851	3.197477
H	-0.936326	0.009751	1.951458
H	-0.936222	0.009764	-0.540726
Li	1.220894	-5.406024	0.706338

Mg^{2+}-Bis(benzene)molybdenum



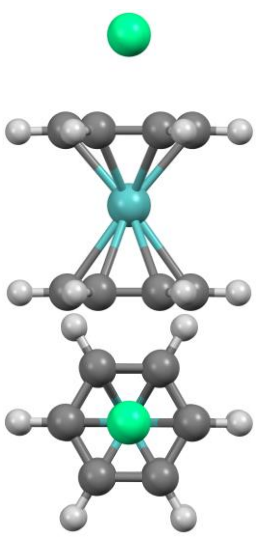
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.408477
C	1.219805	0.000000	2.112590
C	2.439523	-0.000192	1.408215
C	2.439548	-0.000511	-0.000261
C	1.219741	-0.000319	-0.704375
Mo	1.219484	-1.972788	0.704303
C	1.228337	-3.615352	2.158279
C	2.482823	-3.615644	1.423358
C	2.473606	-3.615672	-0.030515
C	1.209888	-3.615539	-0.749451
C	-0.044617	-3.615159	-0.014520
C	-0.035375	-3.614999	1.439369
H	3.405868	-3.609879	-0.576545
H	1.203161	-3.609582	-1.829843
H	-0.983595	-3.608919	-0.548916
H	-0.967632	-3.608658	1.985398
H	1.235065	-3.609322	3.238672
H	3.421799	-3.609865	1.957773
H	1.219754	0.008227	-1.785986
H	3.376313	0.007683	-0.540942
H	3.376183	0.008305	1.949098
H	1.219799	0.008771	3.194199
H	-0.936770	0.008579	1.949144
H	-0.936666	0.008650	-0.540868
Mg	1.218904	-5.537296	0.704692

Na^+-Bis(benzene)molybdenum



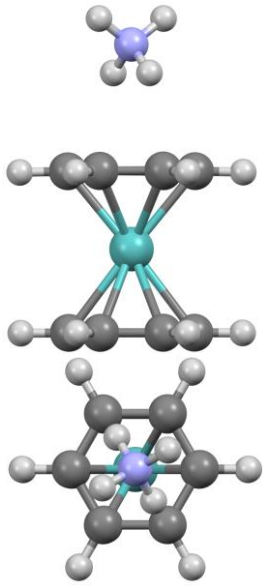
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.411321
C	1.222214	0.000000	2.116938
C	2.444427	0.000277	1.411237
C	2.444427	0.000789	-0.000082
C	1.222211	0.000491	-0.705701
Mo	1.222596	-1.887064	0.705252
C	1.231677	-3.628390	2.136725
C	2.467237	-3.627977	1.413404
C	2.458602	-3.627806	-0.018303
C	1.214444	-3.627810	-0.726735
C	-0.021188	-3.628092	-0.003401
C	-0.012503	-3.628501	1.428370
H	3.391885	-3.603919	-0.564445
H	1.208129	-3.603958	-1.808050
H	-0.960853	-3.604650	-0.538516
H	-0.945790	-3.605236	1.974539
H	1.238005	-3.604866	3.218045
H	3.406879	-3.604256	1.948532
H	1.222360	0.009620	-1.786859
H	3.380808	0.010149	-0.540540
H	3.380698	0.009358	1.951901
H	1.222078	0.008725	3.198100
H	-0.936373	0.008765	1.951804
H	-0.936242	0.008896	-0.540718
Na	1.221474	-5.903914	0.703427

Ca^{2+}-Bis(benzene)molybdenum



C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.407927
C	1.219305	0.000000	2.111836
C	2.438609	0.000213	1.407956
C	2.438633	-0.000000	0.000027
C	1.219338	-0.000213	-0.703905
Mo	1.219315	-1.971148	0.704100
C	1.228741	-3.665797	2.149341
C	2.475463	-3.665876	1.418605
C	2.465988	-3.665847	-0.026502
C	1.209822	-3.665869	-0.740839
C	-0.036921	-3.665571	-0.010092
C	-0.027421	-3.665469	1.435043
H	3.398883	-3.633991	-0.573367
H	1.202636	-3.634324	-1.822192
H	-0.976968	-3.633965	-0.544605
H	-0.960328	-3.633607	1.981893
H	1.235900	-3.633883	3.230677
H	3.415493	-3.633909	1.953112
H	1.219242	0.017372	-1.785349
H	3.375155	0.017643	-0.540778
H	3.375172	0.018034	1.948690
H	1.219401	0.017776	3.193277
H	-0.936520	0.017632	1.948732
H	-0.936572	0.017640	-0.540724
Ca	1.218147	-5.830606	0.703803

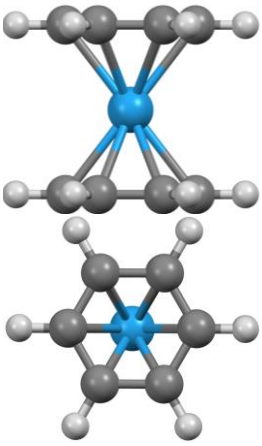
NH_4^+-Bis(benzene)molybdenum



C	-0.002810	-0.197507	-0.000929
C	-0.003758	-0.195635	1.410781
C	1.219885	-0.197447	2.114784
C	2.442522	-0.201050	1.408208
C	2.443471	-0.202850	-0.003502
C	1.219827	-0.201114	-0.707504
Mo	1.223979	1.679002	0.701198
C	2.462639	3.438886	-0.014921
C	1.224728	3.426051	-0.731004
C	-0.009739	3.429670	-0.017397
C	-0.006942	3.446151	1.412687
C	1.230927	3.429755	2.128810
C	2.465384	3.426159	1.415184
H	-0.939847	-0.204773	1.951758
H	1.220884	-0.202867	3.196059
H	3.378860	-0.209226	1.948938
H	3.379507	-0.217505	-0.544448
H	1.218799	-0.209333	-1.788762
H	-0.939178	-0.202975	-0.541642
H	1.228442	3.406691	3.210443
H	-0.943430	3.409534	1.954049
H	-0.948291	3.406526	-0.555035
H	1.227105	3.400125	-1.812573
H	3.398955	3.396764	-0.556180
H	3.403828	3.400302	1.952886
N	1.233627	6.273204	0.695454
H	0.528239	5.635067	1.103065
H	1.653504	6.855577	1.420387
H	1.937325	5.632600	0.288983
H	0.815264	6.855379	-0.030512

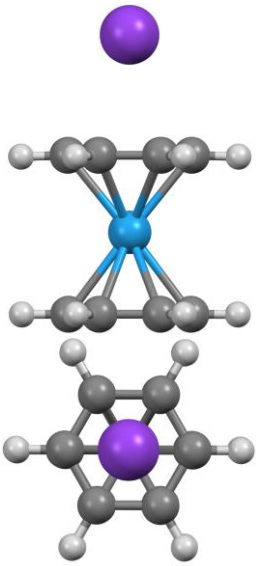
Coordinates for bis(benzene)tungsten and cation-bis(benzene)tungsten complexes

Bis(benzene)tungsten



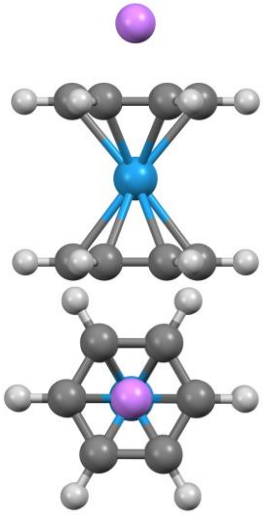
C	-0.004523	0.179853	-0.001870
C	-0.003846	0.179861	1.415648
C	1.224093	0.179730	2.123858
C	2.451387	0.179597	1.414519
C	2.450710	0.179604	-0.002998
C	1.222772	0.179729	-0.711208
W	1.223225	-1.650951	0.706332
C	1.234063	-3.481641	2.123863
C	2.456084	-3.481785	1.405475
C	2.444911	-3.481864	-0.012013
C	1.211772	-3.481719	-0.711106
C	-0.010249	-3.481389	0.007281
C	0.000923	-3.481391	1.424769
H	1.242586	-3.477482	3.205554
H	3.397142	-3.477695	1.938901
H	3.377403	-3.477859	-0.560281
H	1.203251	-3.477625	-1.792798
H	-0.951305	-3.476992	-0.526145
H	-0.931567	-3.477015	1.973038
H	3.388479	0.175244	1.954884
H	1.224627	0.175639	3.205582
H	-0.940369	0.175765	1.956998
H	-0.941616	0.175686	-0.542234
H	1.222237	0.175639	-1.792932
H	3.387232	0.175321	-0.544348

K^+-Bis(benzene)tungsten



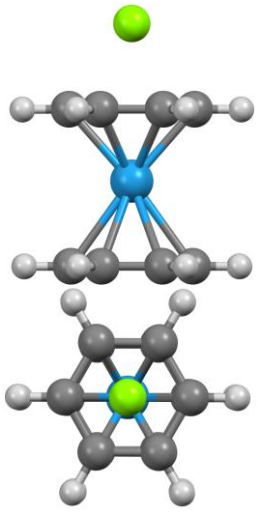
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.413272
C	1.223925	0.000000	2.120019
C	2.447900	0.000085	1.413414
C	2.447925	-0.000171	0.000140
C	1.224009	-0.000278	-0.706630
W	1.223932	-1.883283	0.706829
C	1.232954	-3.654240	2.137061
C	2.466723	-3.654405	1.414339
C	2.457736	-3.654391	-0.015537
C	1.214904	-3.654319	-0.722767
C	-0.018901	-3.654457	0.000006
C	-0.009865	-3.654363	1.429880
H	3.390884	-3.622923	-0.562072
H	1.208071	-3.622832	-1.804167
H	-0.958862	-3.622927	-0.534718
H	-0.942998	-3.622711	1.976408
H	1.239767	-3.622349	3.218432
H	3.406665	-3.622670	1.949063
H	1.224023	0.005263	-1.787731
H	3.384225	0.005363	-0.540364
H	3.384193	0.005792	1.953900
H	1.223920	0.005716	3.201117
H	-0.936296	0.005645	1.953780
H	-0.936364	0.005668	-0.540367
K	1.223970	-6.422879	0.702615

Li^+-Bis(benzene)tungsten



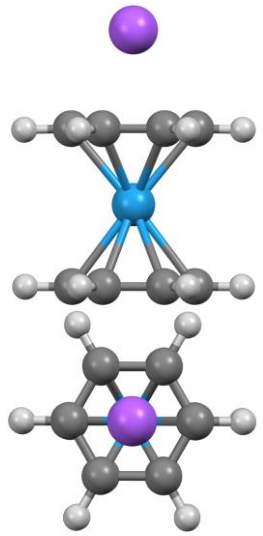
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.412309
C	1.223060	0.000000	2.118529
C	2.446144	0.000384	1.412324
C	2.446144	0.000363	0.000015
C	1.223082	-0.000021	-0.706206
W	1.223358	-1.898572	0.706207
C	1.232494	-3.652640	2.141974
C	2.471169	-3.652668	1.416519
C	2.462294	-3.652821	-0.018932
C	1.214749	-3.652946	-0.729070
C	-0.023940	-3.653221	-0.003577
C	-0.015015	-3.653068	1.431872
H	3.394937	-3.646651	-0.565035
H	1.208057	-3.646935	-1.809811
H	-0.963283	-3.647287	-0.538070
H	-0.947660	-3.647035	1.977974
H	1.239166	-3.646284	3.222714
H	3.410509	-3.646268	1.951013
H	1.223108	0.006203	-1.787241
H	3.382373	0.006896	-0.540469
H	3.382392	0.006918	1.952759
H	1.223045	0.006244	3.199565
H	-0.936222	0.006251	1.952809
H	-0.936273	0.006250	-0.540395
Li	1.223896	-5.428601	0.706202

Mg^{2+}-Bis(benzene)tungsten



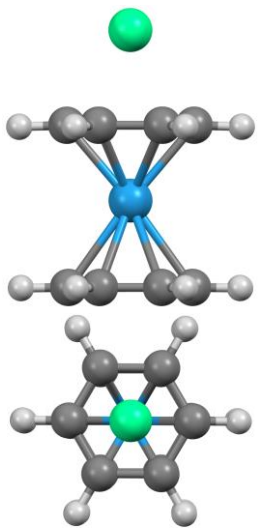
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.410242
C	1.221340	0.000000	2.115326
C	2.442672	0.000043	1.410219
C	2.442672	0.000362	-0.000023
C	1.221332	0.000320	-0.705108
W	1.221519	-1.966131	0.704853
C	1.229632	-3.626147	2.158946
C	2.485190	-3.625910	1.424840
C	2.477214	-3.625742	-0.029592
C	1.213667	-3.625635	-0.749921
C	-0.041878	-3.625850	-0.015822
C	-0.033902	-3.626194	1.438604
H	3.409587	-3.619575	-0.574747
H	1.207810	-3.619372	-1.829956
H	-0.980204	-3.619763	-0.550670
H	-0.966289	-3.620493	1.983747
H	1.235488	-3.620493	3.238989
H	3.423517	-3.619982	1.959692
H	1.221362	0.003664	-1.786654
H	3.379319	0.003803	-0.540786
H	3.379294	0.003197	1.951032
H	1.221300	0.003056	3.196874
H	-0.936650	0.003138	1.951002
H	-0.936624	0.003122	-0.540813
Mg	1.221783	-5.604473	0.704945

Na^+-Bis(benzene)tungsten



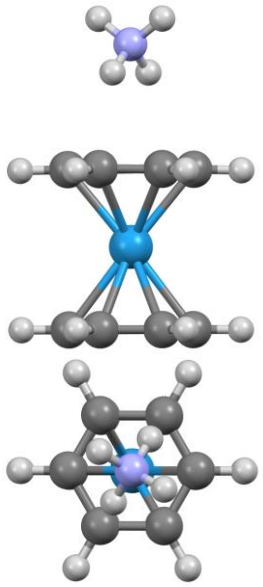
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.412706
C	1.223447	0.000000	2.118978
C	2.446913	0.000555	1.412610
C	2.446937	0.001260	-0.000096
C	1.223502	0.000705	-0.706391
W	1.224174	-1.892174	0.705807
C	1.233772	-3.647985	2.139079
C	2.470876	-3.647160	1.414572
C	2.461936	-3.646804	-0.019058
C	1.215933	-3.647100	-0.728231
C	-0.021216	-3.647687	-0.003669
C	-0.012201	-3.648216	1.429960
H	3.394736	-3.620670	-0.565335
H	1.209309	-3.621238	-1.809202
H	-0.960743	-3.622267	-0.538326
H	-0.945016	-3.623047	1.976251
H	1.240361	-3.622595	3.220056
H	3.410375	-3.621245	1.949249
H	1.223516	0.006420	-1.787409
H	3.383093	0.007464	-0.540662
H	3.383126	0.006164	1.953086
H	1.223440	0.005165	3.199999
H	-0.936149	0.005210	1.953293
H	-0.936231	0.005184	-0.540452
Na	1.225746	-5.928221	0.702419

Ca^{2+}-Bis(benzene)tungsten



C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.409045
C	1.220307	0.000000	2.113561
C	2.440630	0.000149	1.409007
C	2.440630	0.000575	-0.000043
C	1.220317	0.000426	-0.704562
W	1.220598	-1.973120	0.704125
C	1.230728	-3.684155	2.151394
C	2.479223	-3.684005	1.419154
C	2.469332	-3.683451	-0.028198
C	1.210851	-3.683309	-0.743389
C	-0.037711	-3.683875	-0.011050
C	-0.027693	-3.684166	1.436301
H	3.401730	-3.648555	-0.575101
H	1.203391	-3.648569	-1.824344
H	-0.977619	-3.649248	-0.544985
H	-0.960076	-3.649362	1.983220
H	1.238219	-3.649177	3.232326
H	3.419108	-3.649045	1.953095
H	1.220216	0.014174	-1.786004
H	3.377143	0.014446	-0.540798
H	3.377269	0.013761	1.949586
H	1.220393	0.013441	3.195008
H	-0.936512	0.013426	1.949814
H	-0.936636	0.013495	-0.540584
Ca	1.221048	-5.845118	0.701707

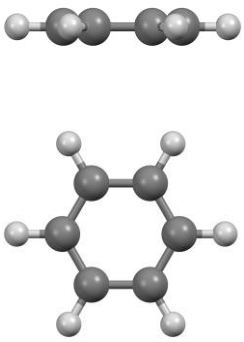
NH_4^+-Bis(benzene)tungsten



C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.413324
C	1.222152	0.000000	2.122665
C	2.449350	0.000000	1.421604
C	2.449362	-0.007925	0.008300
C	1.227224	-0.007925	-0.701063
W	1.227743	1.882011	0.705528
C	2.471342	3.639047	-0.014844
C	1.235912	3.639093	-0.731621
C	-0.004064	3.663831	-0.015821
C	-0.010139	3.647125	1.416031
C	1.225277	3.647100	2.132820
C	2.465346	3.663804	1.416912
H	3.384173	-0.011166	1.964238
H	3.386353	-0.013337	-0.531084
H	1.230796	-0.013335	-1.782206
H	-0.934869	-0.011161	-0.542554
H	-0.936988	0.000656	1.952737
H	1.218661	0.000653	3.203823
H	3.410742	3.611171	-0.550220
H	3.400487	3.620731	1.959640
H	1.226644	3.625271	3.214208
H	-0.949623	3.625290	1.951539
H	-0.939342	3.620778	-0.558313
H	1.234477	3.611196	-1.812869
N	1.235684	6.491139	0.692804
H	1.937697	5.849909	1.102712
H	1.657811	7.070808	-0.033220
H	0.530578	5.851555	0.285829
H	0.816383	7.076146	1.416178

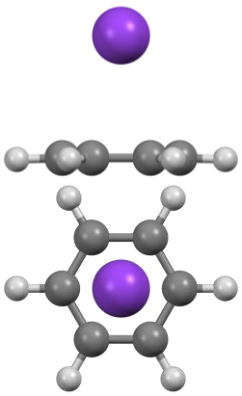
Coordinates for benzene and cation-benzene complexes

Benzene



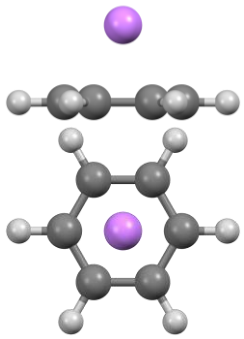
C	-0.000817	0.000000	-0.000471
C	-0.000817	0.000000	1.390471
C	1.203775	0.000000	-0.695943
C	2.408367	0.000000	-0.000471
C	1.203775	0.000000	2.085943
C	2.408367	0.000000	1.390471
H	3.346229	0.000000	1.931946
H	3.346229	0.000000	-0.541946
H	1.203775	0.000000	-1.778892
H	-0.938678	0.000000	-0.541946
H	-0.938678	0.000000	1.931946
H	1.203775	0.000000	3.168892

K^+-Benzene



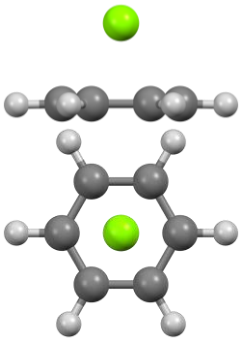
C	-0.003972	0.092291	-0.002296
C	-0.003977	0.092116	1.392993
C	1.204369	0.091771	2.090648
C	2.412725	0.091613	1.392991
C	2.412728	0.091777	-0.002304
C	1.204379	0.092109	-0.699954
H	-0.941258	0.127893	-0.543435
H	-0.941253	0.127590	1.934162
H	1.204380	0.126988	3.172948
H	3.350031	0.126715	1.934141
H	3.350033	0.127000	-0.543445
H	1.204406	0.127575	-1.782242
K	1.206285	-2.815437	0.696447

Li^+-Benzene



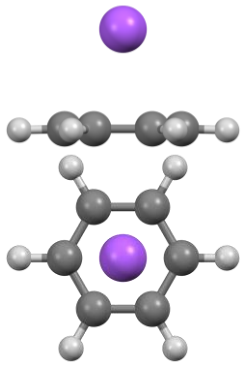
C	-0.006877	0.021860	-0.003987
C	-0.006902	0.021790	1.394809
C	1.204475	0.021667	2.094233
C	2.415883	0.021651	1.394826
C	2.415907	0.021685	-0.003970
C	1.204529	0.021772	-0.703393
H	-0.944144	0.031571	-0.545066
H	-0.944140	0.031430	1.935942
H	1.204496	0.031175	3.176472
H	3.353153	0.031129	1.935908
H	3.353145	0.031210	-0.545107
H	1.204506	0.031395	-1.785631
Li	1.204844	-1.818334	0.695618

Mg^{2+}-Benzene



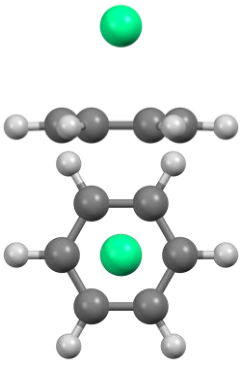
C	-0.018226	0.022045	-0.010495
C	-0.018233	0.021989	1.401395
C	1.204534	0.021891	2.107314
C	2.427285	0.021862	1.401365
C	2.427291	0.021897	-0.010528
C	1.204522	0.021982	-0.716444
H	-0.957191	0.045195	-0.552627
H	-0.957216	0.045102	1.943502
H	1.204521	0.044928	3.191552
H	3.366254	0.044872	1.943499
H	3.366277	0.044940	-0.552632
H	1.204539	0.045090	-1.800680
Mg	1.204521	-1.901793	0.695431

Na^+-Benzene



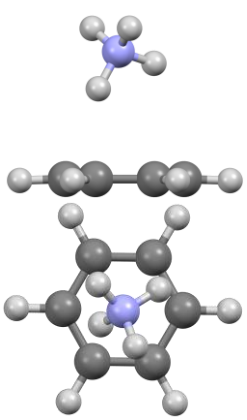
C	-0.005552	0.055306	-0.003237
C	-0.005529	0.055222	1.393989
C	1.204487	0.055033	2.092635
C	2.414497	0.054928	1.394040
C	2.414473	0.055030	-0.003191
C	1.204451	0.055221	-0.701832
H	-0.942776	0.085162	-0.544343
H	-0.942750	0.085021	1.935107
H	1.204501	0.084708	3.174856
H	3.351728	0.084535	1.935153
H	3.351701	0.084706	-0.544307
H	1.204442	0.085027	-1.784047
Na	1.205202	-2.339899	0.695828

Ca^{2+}-Benzene



C	-0.011496	0.047564	-0.006651
C	-0.011486	0.047501	1.397481
C	1.204507	0.047411	2.099566
C	2.420503	0.047322	1.397491
C	2.420492	0.047381	-0.006643
C	1.204499	0.047531	-0.708727
H	-0.949971	0.087620	-0.548479
H	-0.949957	0.087508	1.939322
H	1.204502	0.087336	3.183233
H	3.358986	0.087190	1.939323
H	3.358973	0.087293	-0.548476
H	1.204514	0.087550	-1.792389
Ca	1.204812	-2.309207	0.695599

NH_4^+-Benzene



C	-0.013611	0.095012	0.003798
C	0.000833	0.035751	1.396047
C	1.216668	-0.041365	2.077743
C	2.417685	-0.055585	1.363784
C	2.400911	0.006786	-0.030540
C	1.185873	0.080495	-0.709102
H	1.173940	0.159960	-1.788951
H	3.332277	0.027819	-0.582112
H	3.361645	-0.078510	1.894085
H	-0.954969	0.185574	-0.523575
H	-0.928075	0.079214	1.950465
H	1.231176	-0.052520	3.160572
N	1.177116	-2.997366	0.716613
H	0.712582	-2.666617	-0.133689
H	1.477315	-2.149142	1.239697
H	1.988932	-3.566746	0.471355
H	0.524882	-3.546638	1.279002