Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Exotic species with explicit

Noble metal–Noble gas–Noble metal linkages

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Supplementary Information

Cartesian Coordinates for All Structures Reported in This Work

Structures optimized at the CCSD/SDDALL level.

$\mathbf{Pt_2Ng_2F_4}$ ($D_{2h,a}$)

	$Pt_2Kr_2F_4$			
1.	Pt	1.667647	0.000004	-0.090395
2.	F	2.920876	-1.444961	-0.452653
3.	F	2.920841	1.444974	-0.452758
4.	Pt	-1.667649	-0.000003	-0.090389
5.	F	-2.920838	-1.444974	-0.452761
6.	F	-2.920877	1.444957	-0.452668
7.	Kr	-0.000004	2.065589	0.422202
8.	Kr	0.000007	-2.065589	0.422206

	$Pt_2Xe_2F_4$			
1.	Pt	-1.900407	0.000078	-0.000009
2.	F	-3.230291	-1.436166	0.000006
3.	F	-3.230174	1.436448	-0.000104
4.	Pt	1.900281	-0.000123	-0.000068
5.	F	3.230108	-1.436437	-0.000001
6.	F	3.230451	1.435864	-0.000382
7.	Xe	0.000305	2.028339	-0.000027
8.	Xe	-0.000138	-2.028226	0.000217

$Pt_2Rn_2F_4$				
1.	Pt	-1.942287	-0.000598	0.000138
2.	F	-3.272998	1.433101	0.000367
3.	F	-3.272043	-1.435184	0.000126
4.	Pt	1.942281	0.000520	-0.000180
5.	F	3.272136	1.435012	-0.000239
6.	F	3.272987	-1.433165	-0.000304
7.	Rn	0.000689	-2.204269	-0.000292
8.	Rn	-0.000692	2.204364	0.000335

$[Au_2Ng_2F_4]^{+2}$ ($D_{2h,a}$)

$[Au_2Kr_2F_4]^{+2}$				
1.	Au	2.136733	0.000021	-0.000334
2.	F	3.501456	-1.380991	0.000404
3.	F	3.501394	1.381088	0.000074
4.	Au	-2.136721	-0.000021	0.000193
5.	F	-3.501380	-1.381090	-0.000058
6.	F	-3.501445	1.380990	0.000194
7.	Kr	-0.000098	1.941845	0.000107
8.	Kr	0.000067	-1.941844	0.000049

$[Au_2Xe_2F_4]^{+2}$				
1.	Au	-2.024999	-0.000053	-0.000131
2.	F	-3.401039	1.373010	-0.000035
3.	F	-3.400850	-1.373300	-0.000346
4.	Au	2.025095	0.000055	0.000142
5.	F	3.400929	1.373315	0.000364
6.	F	3.401103	-1.373034	-0.000018
7.	Xe	0.000053	-2.082562	-0.000308
8.	Xe	-0.000217	2.082561	0.000298

	$[Au_2Rn_2F_4]^{+2}$			
1.	Au	-2.019631	-0.000104	-0.000108
2.	F	-3.398084	-1.373179	-0.000136
3.	F	-3.398258	1.372800	-0.000129
4.	Au	2.019500	0.000104	0.000068
5.	F	3.398195	-1.372740	0.000146
6.	F	3.398014	1.373128	0.000022
7.	Rn	-0.000071	2.207878	-0.000023
8.	Rn	0.000205	-2.207878	0.000070

$[AuXe_4]^{+2}$ (D_{4h})

1.	Au	0.000000	0.000000	0.000000
2.	Xe	0.000000	2.821733	0.000000
3.	Xe	2.821733	0.000000	0.000000
4.	Xe	0.000000	-2.821733	0.000000
5.	Xe	-2.821733	0.000000	0.000000

Structures optimized at the MP2/SDDALL level.

$Pt_2Ng_2F_4$ ($D_{2h,a}$)

$Pt_2Kr_2F_4$				
1.	Pt	1.607300	-0.000003	-0.096407
2.	F	2.875158	-1.417327	-0.498488
3.	F	2.875151	1.417327	-0.498492
4.	Pt	-1.607295	-0.000005	-0.096405
5.	F	-2.875158	-1.417321	-0.498497
6.	F	-2.875163	1.417306	-0.498499
7.	Kr	-0.000008	2.029829	0.458125
8.	Kr	-0.000002	-2.029808	0.458130

$Pt_2Xe_2F_4$				
1.	Pt	-1.861273	0.000009	-0.000022
2.	F	-3.213174	-1.412589	-0.000094
3.	F	-3.213168	1.412605	0.000121
4.	Pt	1.861291	-0.000015	-0.000059
5.	F	3.213079	-1.412746	0.000080
6.	F	3.213167	1.412573	0.000132
7.	Xe	0.000032	1.975866	0.000023
8.	Xe	-0.000041	-1.975831	0.000055

$Pt_2Rn_2F_4$

1.	Pt	-1.900612	-0.000799	0.000275
2.	F	-3.252411	1.410499	0.001363
3.	F	-3.251148	-1.413319	0.000651
4.	Pt	1.900695	0.000782	0.000649
5.	F	3.251210	1.413288	0.000599
6.	F	3.252453	-1.410540	-0.000483
7.	Rn	0.000935	-2.171867	-0.000469
8.	Rn	-0.001022	2.171890	-0.000592

$[Au_2Ng_2F_4]^{+2}$ ($D_{2h,a}$)

$[Au_2Kr_2F_4]^{+2}$

1.	Au	-2.040537	-0.000015	0.000014
2.	F	-3.423672	1.384089	0.000132
3.	F	-3.423598	-1.384188	0.000124
4.	Au	2.040518	0.000015	0.000017
5.	F	3.423598	1.384170	0.000118
6.	F	3.423640	-1.384102	0.000125
7.	Kr	0.000087	-1.922108	-0.000097
8.	Kr	-0.000037	1.922116	-0.000097

$[Au_2Xe_2F_4]^{+2}$

1.	Au	-1.959030	-0.000017	0.000081
2.	F	-3.356514	1.379673	0.000544
3.	F	-3.356460	-1.379742	0.000405
4.	Au	1.959027	0.000005	0.000298
5.	F	3.356464	1.379741	0.001304
6.	F	3.356508	-1.379670	0.000409
7.	Xe	0.000031	-2.067453	-0.000630
8.	Xe	-0.000027	2.067471	-0.000368

$[Au_2Rn_2F_4]^{+2}$

1.	Au	-1.962191	-0.000687	0.000233
2.	F	-3.360969	-1.383473	0.000515
3.	F	-3.362081	1.380962	0.000743
4.	Au	1.962091	0.000648	0.000189
5.	F	3.361935	-1.381104	0.000770
6.	F	3.360981	1.383286	0.000712
7.	Rn	-0.000799	2.205480	-0.000343
8.	Rn	0.000905	-2.205410	-0.000332

$[AuXe_4]^{+2}$ (D_{4h})

1.	Au	0.000000	0.000000	0.000000
2.	Xe	2.784774	0.000000	0.000000
3.	Xe	0.000000	2.784774	0.000000
4.	Xe	-2.784774	0.000000	0.000000
5.	Xe	0.000000	-2.784774	0.000000

QTAIM: Bonding Critical Points for Structures $D_{2h,a}$ Reported in This Work

$Pt_2Ng_2F_4$

$Pt_2Kr_2F_4$

BCP #	Name	Atoms	ρ	$\nabla^2\rho$	V	G	H	| V/G |
1	BCP1	Pt1-Kr8	0.043	0.179	-0.056	0.050	-0.006	1.114
2	BCP2	Pt1-F2	0.119	0.576	-0.177	0.160	-0.017	1.104
3	BCP3	Pt1-Kr7	0.043	0.179	-0.056	0.050	-0.006	1.114
4	BCP4	Pt1-F3	0.119	0.576	-0.177	0.160	-0.017	1.104
5	BCP5	Pt1-Pt4	0.023	0.059	-0.016	0.016	-0.001	1.044
6	BCP6	Pt4-Kr8	0.043	0.179	-0.056	0.050	-0.006	1.114
7	BCP7	Pt4-F5	0.119	0.576	-0.177	0.160	-0.017	1.104
8	BCP8	Pt4-Kr7	0.043	0.179	-0.056	0.050	-0.006	1.114
9	BCP9	Pt4-F6	0.119	0.576	-0.177	0.160	-0.017	1.104

$Pt_2Xe_2F_4$

BCP #	Name	Atoms	ρ	$\nabla^2\rho$	V	G	H	| V/G |
1	BCP1	Pt1-Xe8	0.052	0.162	-0.062	0.051	-0.011	1.211
2	BCP2	Pt1-F2	0.116	0.563	-0.171	0.156	-0.015	1.099
3	BCP3	Pt1-Xe7	0.052	0.162	-0.062	0.051	-0.011	1.211
4	BCP4	Pt1-F3	0.116	0.563	-0.171	0.156	-0.015	1.099
5	BCP5	Pt4-Xe8	0.052	0.162	-0.062	0.051	-0.011	1.211
6	BCP6	Pt4-F5	0.116	0.563	-0.171	0.156	-0.015	1.099
7	BCP7	Pt4-Xe7	0.052	0.162	-0.062	0.051	-0.011	1.211
8	BCP8	Pt4-F6	0.116	0.563	-0.171	0.156	-0.015	1.099

$Pt_2Rn_2F_4$

BCP #	Name	Atoms	ρ	$\nabla^2\rho$	V	G	H	| V/G |
1	BCP1	Pt1-Rn8	0.040	0.117	-0.042	0.035	-0.007	1.201
2	BCP2	Pt1-F2	0.115	0.567	-0.171	0.156	-0.015	1.096
3	BCP3	Pt1-Rn7	0.040	0.117	-0.042	0.035	-0.007	1.201
4	BCP4	Pt1-F3	0.115	0.567	-0.171	0.156	-0.015	1.096
5	BCP5	Pt4-Rn8	0.040	0.117	-0.042	0.035	-0.007	1.201
6	BCP6	Pt4-F5	0.115	0.567	-0.171	0.156	-0.015	1.096
7	BCP7	Pt4-Rn7	0.040	0.117	-0.042	0.035	-0.007	1.201
8	BCP8	Pt4-F6	0.115	0.567	-0.171	0.156	-0.015	1.096

$[Au_2Ng_2F_4]^{+2}$

$[Au_2Kr_2F_4]^{+2}$

BCP #	Name	Atoms	ρ	$\nabla^2\rho$	V	G	H	| V/G |
1	BCP1	Au1-Kr8	0.035	0.115	-0.035	0.032	-0.003	1.102
2	BCP2	Au1-F2	0.116	0.525	-0.157	0.144	-0.013	1.092
3	BCP3	Au1-Kr7	0.035	0.115	-0.035	0.032	-0.003	1.102
4	BCP4	Au1-F3	0.116	0.525	-0.157	0.144	-0.013	1.092
5	BCP5	Au4-Kr8	0.035	0.115	-0.035	0.032	-0.003	1.102
6	BCP6	Au4-F5	0.116	0.525	-0.157	0.144	-0.013	1.092
7	BCP7	Au4-Kr7	0.035	0.115	-0.035	0.032	-0.003	1.102
8	BCP8	Au4-F6	0.116	0.525	-0.157	0.144	-0.013	1.092

$[Au_2Xe_2F_4]^{+2}$

BCP #	Name	Atoms	ρ	$\nabla^2\rho$	V	G	H	| V/G |
1	BCP1	Au1-Xe8	0.044	0.103	-0.041	0.033	-0.007	1.224
2	BCP2	Au1-F2	0.115	0.517	-0.155	0.142	-0.013	1.093
3	BCP3	Au1-Xe7	0.044	0.103	-0.041	0.033	-0.007	1.224
4	BCP4	Au1-F3	0.115	0.517	-0.155	0.142	-0.013	1.093
5	BCP5	Au4-Xe8	0.044	0.103	-0.041	0.033	-0.007	1.224
6	BCP6	Au4-F5	0.115	0.517	-0.155	0.142	-0.013	1.093
7	BCP7	Au4-Xe7	0.044	0.103	-0.041	0.033	-0.007	1.224
8	BCP8	Au4-F6	0.115	0.517	-0.155	0.142	-0.013	1.093

$[Au_2Rn_2F_4]^{+2}$

BCP #	Name	Atoms	ρ	$\nabla^2\rho$	V	G	H	| V/G |
1	BCP1	Au1-Rn8	0.041	0.083	-0.032	0.026	-0.007	1.254
2	BCP2	Au1-F2	0.114	0.519	-0.155	0.142	-0.013	1.089
3	BCP3	Au1-Rn7	0.041	0.083	-0.032	0.026	-0.007	1.254
4	BCP4	Au1-F3	0.114	0.519	-0.155	0.142	-0.013	1.089
5	BCP5	Au4-Rn8	0.041	0.083	-0.033	0.026	-0.007	1.254
6	BCP6	Au4-F5	0.114	0.519	-0.155	0.142	-0.013	1.089
7	BCP7	Au4-Rn7	0.041	0.083	-0.032	0.026	-0.007	1.254
8	BCP8	Au4-F6	0.114	0.519	-0.155	0.142	-0.013	1.089

$[AuXe_4]^{+2}$ (D_{4h})

BCP #	Name	Atoms	ρ	$\nabla^2\rho$	V	G	H	| V/G |
1	BCP1	Au1-Rn8	0.041	0.083	-0.032	0.026	-0.007	1.254
2	BCP2	Au1-F2	0.114	0.519	-0.155	0.142	-0.013	1.089
3	BCP3	Au1-Rn7	0.041	0.083	-0.032	0.026	-0.007	1.254
4	BCP4	Au1-F3	0.114	0.519	-0.155	0.142	-0.013	1.089

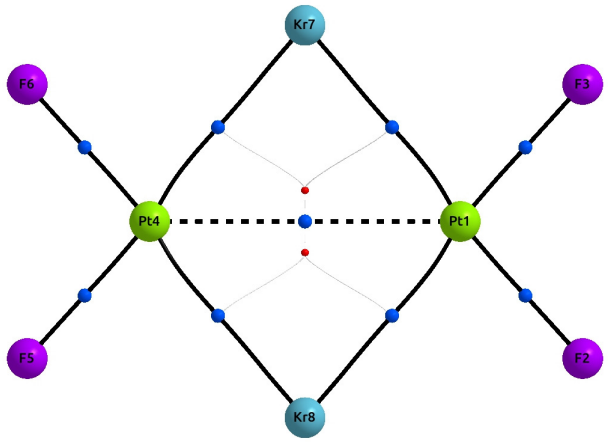

Figure 1: Molecular graphs for the $Pt_2Kr_2F_4$ species.