

Probing the reactions of thiourea ($\text{CH}_4\text{N}_2\text{S}$) with metals ($\text{X} = \text{Au, Hf, Hg, Ir, Os, W, Pt, and Re}$) anchored fullerene surfaces (C_{59}X)

Hitler Louis ^{a,b}, Destiny E. Charlie ^{a,b}, Ismail O. Amodu ^{a,c}, Innocent Benjamin ^a,
Terkumur E. Gber ^{a,b} and Adedapo S. Adeyinka ^{d*}**

^aComputational and Bio-Simulation Research Group, University of Calabar, Calabar, Nigeria

^bDepartment of Pure and Applied Chemistry, Faculty of Physical Sciences, University of Calabar, Calabar, Nigeria

^cDepartment of Mathematics, Faculty of Physical Sciences, University of Calabar, Calabar, Nigeria

^dDepartment of Chemical Sciences, University of Johannesburg, South-Africa-2006

*Corresponding authors' email: louismuzong@gmail.com and aadeyinka@uj.ac.za

Table S1: the result of the other observed charge transfer associated with higher perturbation energy.

Compound	Donor	Acceptor	E ²	E(i)-E(j)	F(i,j)
C ₅₉ Au	$\pi^*C_{46}-C_{47}$	$\pi^*C_{41}-C_{42}$	250.1	0.01	0.081
	$\pi^*C_{44}-C_{56}$	$\pi^*C_{54}-C_{55}$	207.09	0.01	0.078
	$\pi^*C_{46}-C_{47}$	$\pi^*C_{40}-C_{48}$	186.52	0.02	0.084
	$\pi^*C_{46}-C_{47}$	$\pi^*C_{51}-C_{52}$	142.62	0.02	0.079
	LP C ₅₃	$\pi^*C_{61}-S_{68}$	113.29	0.16	0.130
C ₅₉ Hf	$\pi^*C_{50}-C_{51}$	$\pi^*C_{44}-C_{52}$	329.59	0.01	0.085
	$\pi^*C_{32}-C_{33}$	$\pi^*C_{30}-C_{31}$	316.62	0.01	0.082
	$\pi^*C_{50}-C_{51}$	$\pi^*C_{45}-C_{46}$	201.61	0.01	0.081
	$\pi^*C_{28}-C_{29}$	$\pi^*C_{30}-C_{31}$	134.82	0.02	0.081
	$\pi^*C_{32}-C_{33}$	$\pi^*C_{30}-C_{31}$	134.62	0.02	0.081
	Lp*C ₂₇	πC_8-C_{26}	114.88	0.14	0.111
C ₅₉ Hg	LP*C ₃₅	$\sigma^*C_{35}-Hg_{60}$	352.99	0.09	0.253
	$\pi^*C_{26}-C_{27}$	$\pi^*C_{28}-C_{29}$	241.48	0.02	0.084
	LP Hg ₆₀	LP*C ₃₅	228.33	1.02	0.482
	$\pi^*C_{24}-C_{25}$	$\pi^*C_{22}-C_{23}$	199.59	0.02	0.083
	$\pi^*C_{24}-C_{25}$	$\pi^*C_{10}-C_{11}$	189.31	0.02	0.084
	LP*C ₃₅	$\sigma^*C_{34}-Hg_{60}$	125.54	1.67	0.665
C ₅₉ Ir	$\sigma C_{35}-Ir_{60}$	$\sigma^*C_{27}-Ir_{60}$	157.69	2.15	0.750
	$\sigma C_{27}-Ir_{60}$	$\sigma^*C_{35}-Ir_{60}$	151.90	2.39	0.780
	$\sigma C_{27}-Ir_{60}$	$\sigma^*C_{34}-Ir_{60}$	146.62	2.11	0.722
	$\sigma C_{35}-Ir_{60}$	$\sigma^*C_{27}-Ir_{60}$	128.12	2.42	0.717
	$\pi^*C_{35}-Ir_{60}$	$\pi^*C_{26}-C_{27}$	114.62	0.03	0.089
	$\sigma C_{27}-Ir_{60}$	$\sigma^*C_{27}-Ir_{60}$	104.11	2.11	0.608
C ₅₉ Os	$\pi^*C_{22}-C_{23}$	$\pi^*C_{20}-C_{21}$	286.29	0.01	0.081
	$\pi^*C_{24}-C_{25}$	$\pi^*C_{10}-C_{11}$	268.30	0.01	0.085
	$\sigma C_{35}-Os_{60}$	$\sigma^*C_{27}-Os_{60}$	196.40	2.00	0.568
	$\sigma C_{35}-Os_{60}$	$\sigma^*C_{34}-Os_{60}$	196.27	2.00	0.568
	$\sigma C_{27}-Os_{60}$	$\sigma^*C_{35}-Os_{60}$	188.50	2.23	0.592
C ₅₉ Pt	$\sigma C_{27}-Pt_{60}$	LP*C ₃₅	971.84	0.69	0.865
	$\sigma C_{27}-Pt_{60}$	$\sigma^*C_{34}-Pt_{60}$	600.97	2.63	1.135
	$\sigma C_{27}-Pt_{60}$	$\sigma^*C_{27}-Pt_{60}$	425.46	2.63	0.955
	LP Pt ₆₀	LP*C ₃₅	413.13	0.70	0.545
	LP* C ₃₅	$\sigma^*C_{27}-Pt_{60}$	369.79	1.94	1.044
	$\sigma C_{27}-Pt_{60}$	LP* C ₃₅	174.05	1.10	0.403
C ₅₉ Re	$\sigma C_{35}-Re_{60}$	$\sigma^*C_{34}-Re_{60}$	814.61	0.37	1.727
	$\sigma^*C_{34}-Re_{60}$	$\sigma^*C_{35}-Re_{60}$	674.89	0.33	1.270
	$\sigma^*C_{34}-Re_{60}$	LP*Re ₆₀	355.10	0.69	1.590
	$\sigma^*C_{27}-Re_{60}$	LP*Re ₆₀	354.59	0.69	1.586
	$\sigma^*C_{22}-C_{23}$	$\sigma^*C_{34}-Re_{60}$	146.91	0.01	0.
	$\sigma C_{35}-Re_{60}$	$\sigma^*C_{34}-Re_{60}$	124.39	2.04	0.646
C ₅₉ W	$\pi C_{34}-W_{60}$	LP* C ₄₉	581.56	0.04	0.170

	π C ₂₇ -W ₆₀	LP C ₂₆	580.71	0.04	0.170
	π^* C ₂₂ -C ₂₃	π^* C ₂₀ -C ₂₁	309.93	0.01	0.083
	π C ₂₇ -W ₆₀	π^* C ₃₄ -W ₆₀	216.10	0.76	0.385
	π C ₂₇ -W ₆₀	σ C ₃₅ -W ₆₀	204.15	0.98	0.428
TOU@C ₅₉ Au	σ N ₆₂ -H ₆₃	π^* C ₆₁ -N ₆₂	196.68	0.96	0.587
	σ N ₆₂ -H ₆₄	π^* C ₆₁ -N ₆₂	168.05	0.99	0.557
	π^* C ₂₈ -C ₂₉	π^* C ₇ -C ₈	158.40	0.01	0.084
	σ C ₃₄ -Au ₆₀	LP* Au ₆₀	133.16	0.06	0.153
	LP S ₆₈	σ^* Au ₆₀ -S ₆₈	148.67	0.80	0.435
TOU@C ₅₉ Hf	σ^* C ₃₄ -Hf ₆₀	σ^* C ₂₇ -Hf ₆₀	691.11	0.03	0.347
	σ^* C ₂₇ -Hf ₆₀	σ^* C ₃₅ -Hf ₆₀	275.15	0.09	0.377
	σ^* C ₂₇ -Hf ₆₀	σ^* Hf ₆₀ -S ₆₈	267.85	0.06	0.344
	π^* C ₃₂ -C ₃₃	π^* C ₃₀ -C ₃₁	256.85	0.01	0.083
	π^* C ₃₂ -C ₃₃	π^* C ₅₀ -C ₅₁	247.36	0.01	0.082
TOU@C ₅₉ Hg	π^* C ₂₈ -C ₂₉	π^* C ₃₀ -C ₃₁	280.31	0.01	0.084
	π^* C ₃₂ -C ₃₃	π^* C ₃₀ -C ₃₁	265.06	0.01	0.084
	π^* C ₂₈ -C ₂₉	π^* C ₇ -C ₈	209.47	0.01	0.081
	π^* C ₃₂ -C ₃₃	π^* C ₅₀ -C ₅₁	203.86	0.01	0.081
	LP C ₃₅	LP* Hg ₆₀	112.75	0.46	0.206
TOU@C ₅₉ Ir	π^* C ₂₈ -C ₂₉	π^* C ₂₆ -C ₂₇	114.41	0.01	0.085
	π^* C ₃₂ -C ₃₃	π^* C ₃₄ -C ₄₉	114.41	0.01	0.085
	π^* C ₂₄ -C ₂₅	π^* C ₂₆ -C ₂₇	65.67	0.02	0.075
	π^* C ₃₆ -C ₄₈	π^* C ₃₄ -C ₄₉	65.65	0.02	0.075
	σ^* C ₃₅ -Ir ₆₀	BD*(3)Ir ₆₀ -S ₆₂	39.82	0.20	0.363
TOU@C ₅₉ Os	π^* C ₃₅ -Os ₆₀	σ^* Os ₆₀ -S ₆₈	200.47	0.17	0.400
	σ^* C ₃₄ -Os ₆₀	σ^* Os ₆₀ -S ₆₈	165.59	0.19	0.399
	σ^* C ₂₇ -Os ₆₀	σ^* Os ₆₀ -S ₆₈	165.42	0.19	0.399
	LP Os ₆₀	π^* C ₃₅ -C ₃₆	136.00	0.27	0.174
	σ C ₂₇ -Os ₆₀	σ^* C ₂₇ -Os ₆₀	101.37	1.06	0.200
TOU@C ₅₉ Pt	LP Pt ₆₀	LP*S ₆₂	572.76	0.17	0.321
	π^* C ₃₉ -C ₄₇	π^* C ₄₅ -C ₄₆	237.58	0.01	0.082
	π^* C ₁₀ -C ₁₁	π^* C ₄ -C ₉	237.51	0.01	0.082
	σ C ₃₅ -Pt ₆₀	LP Pt ₆₀	141.37	0.13	0.171
	LP Pt ₆₀	π^* C ₆₁ -S ₆₂	136.41	0.42	0.222
TOU@C ₅₉ Re	σ C ₆₁ -N ₆₂	BD*(3)C ₆₁ -S ₆₈	156.16	1.43	0.618
	σ C ₂₇ -Re ₆₀	σ^* C ₃₄ -Re ₆₀	138.14	1.35	0.557
	σ C ₃₄ -Re ₆₀	σ^* C ₂₇ -Re ₆₀	136.45	1.35	0.553
	σ C ₂₇ -Re ₆₀	σ^* C ₃₅ -Re ₆₀	124.63	1.07	0.475
	σ C ₃₄ -Re ₆₀	σ^* C ₃₅ -Re ₆₀	124.05	1.07	0.474
TOU@C ₅₉ W	π^* C ₃₅ -W ₆₀	π^* C ₃₆ -C ₄₈	257.07	0.01	0.083
	π^* C ₃₅ -W ₆₀	π^* C ₂₄ -C ₂₅	257.06	0.01	0.083

	$\sigma^*C_{27}-W_{60}$	$\sigma^*W_{60}-S_{62}$	193.32	0.51	0.803
	$\sigma^*C_{34}-W_{60}$	$\sigma^*W_{60}-S_{62}$	193.27	0.51	0.803
	$\sigma^*C_{35}-W_{60}$	$\sigma^*W_{60}-S_{62}$	140.09	0.57	0.744