Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Theoretical and Experimental Studies of the Interactions between Au_2^- and Nucleobases

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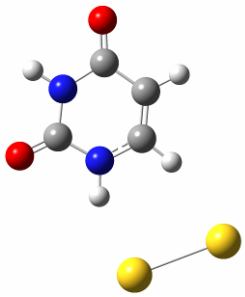
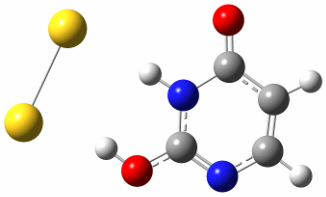
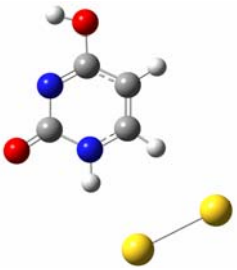
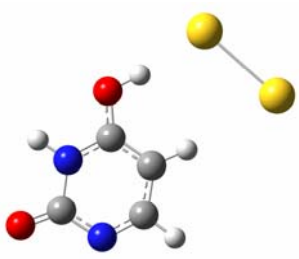
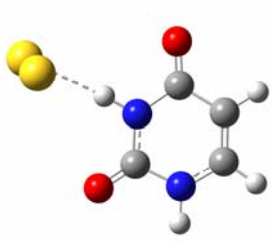
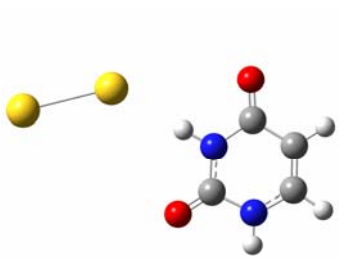
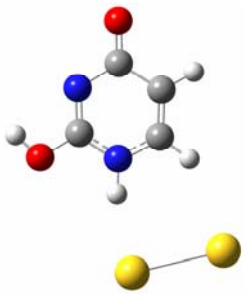
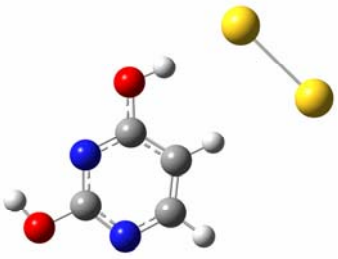
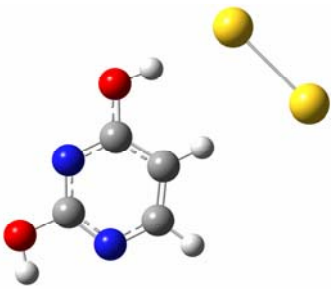
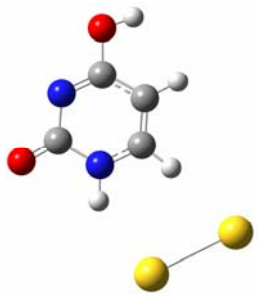
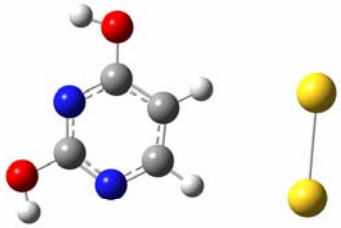
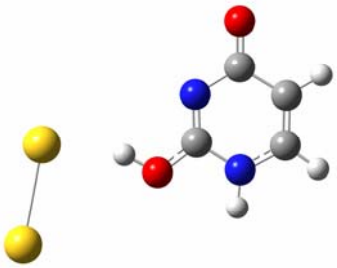
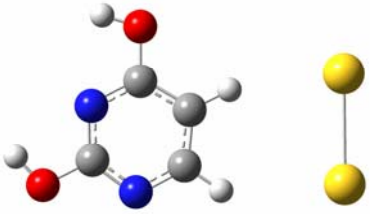
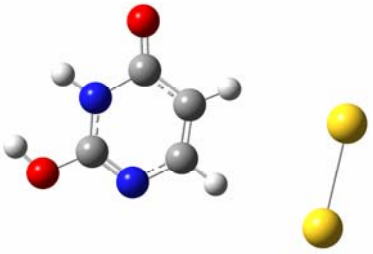
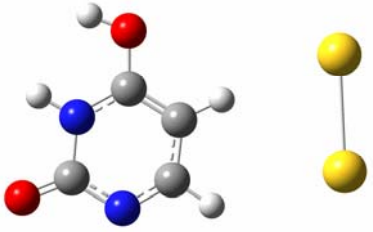
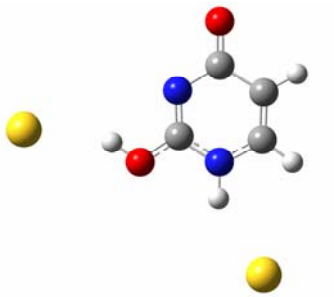
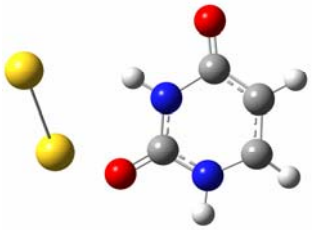
Table S1 The optimized structures, VDEs, and ADEs of UAu_2^- for all the tautomers of uracil*. The VDEs and ADEs were not calculated when the isomers are higher than the lowest-energy structure by more than 0.76 eV.

ΔE	Structures	VDE	ADE
0		2.91	2.25
0.57		3.03	2.87
0.60		2.82	2.02
0.64		3.18	2.95

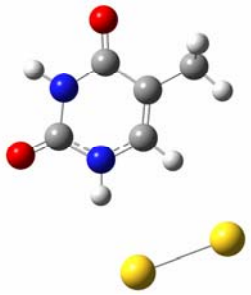
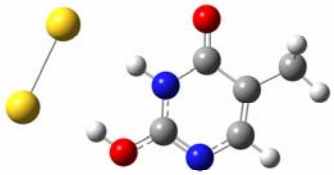
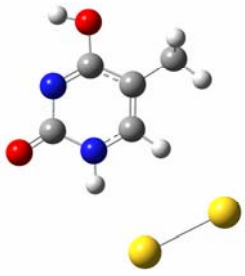
0.71		2.24	1.53
0.74		2.24	1.50
0.76		2.96	2.65
0.78			
0.80			

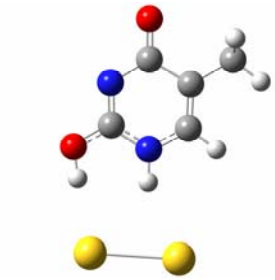
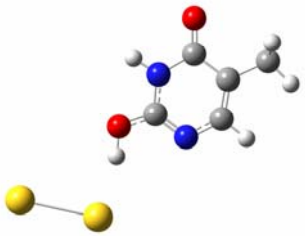
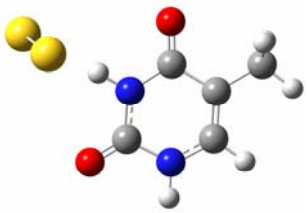
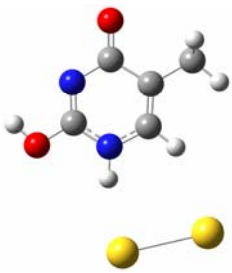
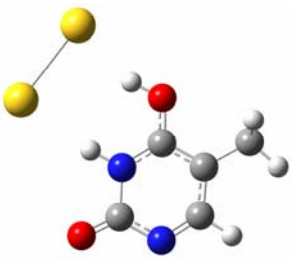
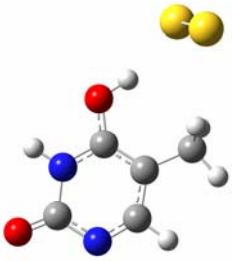
0.86			
1.09			
1.14			
1.17			
1.44			
1.51			

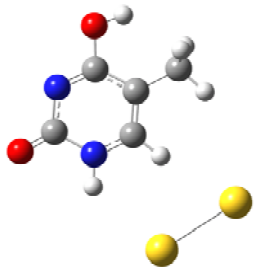
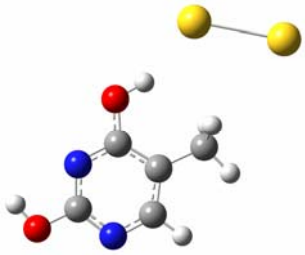
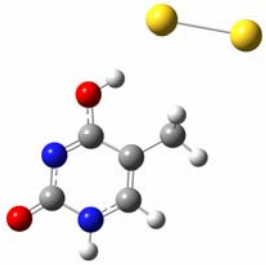
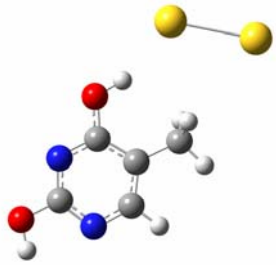
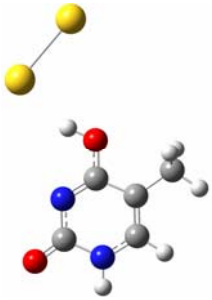
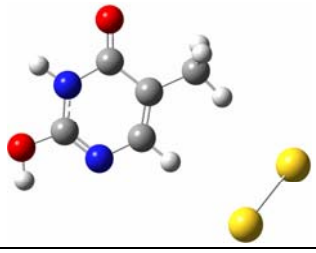
1.69		3.81	3.22
3.08 (spin=3)			

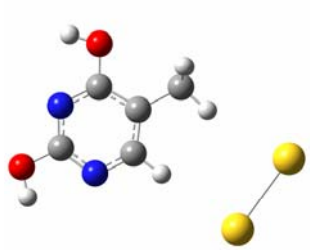
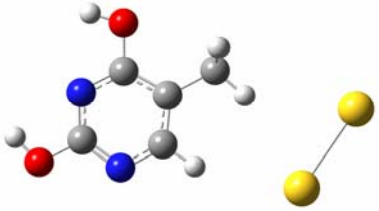
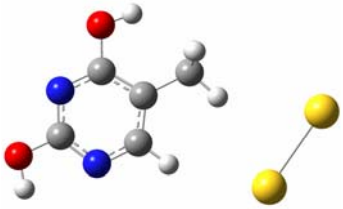
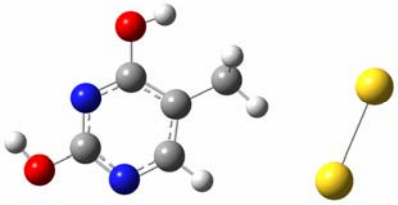
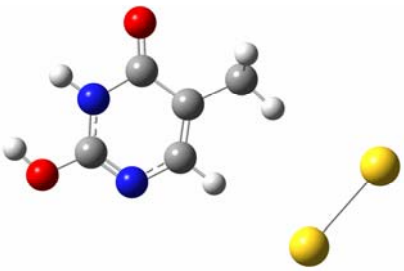
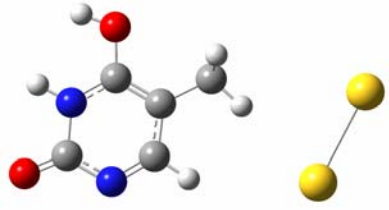
*The energies are in eV.

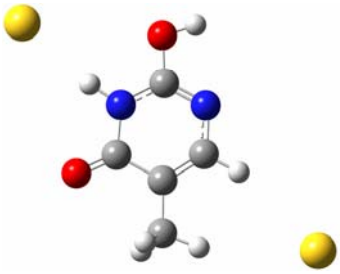
Table S2 The optimized structures, VDEs, and ADEs of TAu_2^- for all the tautomers of thymine*.

ΔE	The optimized structures	VDE	ADE
0		2.88	2.19
0.55		3.01	2.31
0.62		2.80	1.97

0.63		3.42	3.23
0.65		2.69	1.68
0.69		2.24	1.51
0.73			
0.75			
0.79			

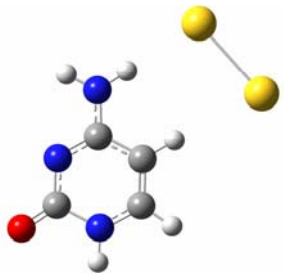
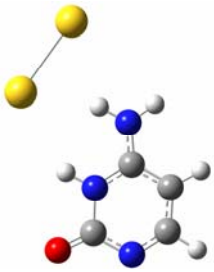
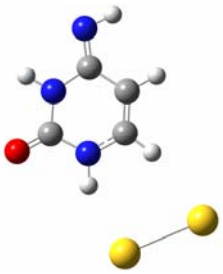
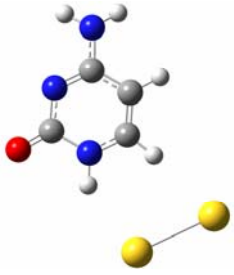
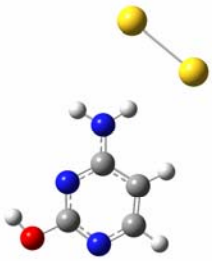
0.88			
0.93			
0.94			
0.96			
0.97			
1.02			

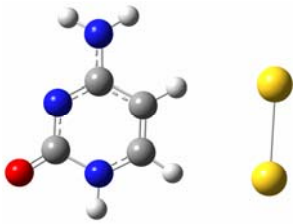
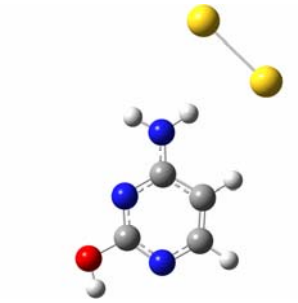
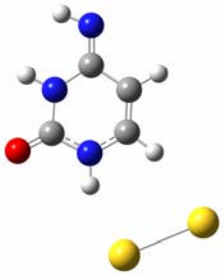
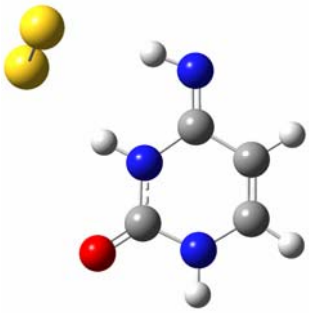
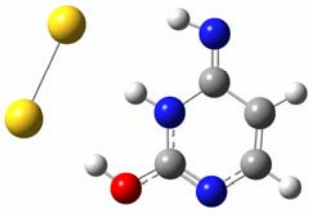
1.10			
1.19			
1.20			
1.24			
1.40			
1.60			

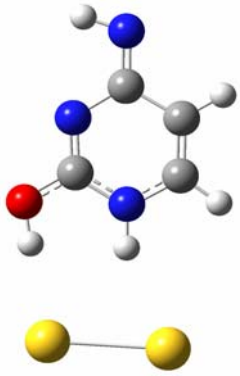
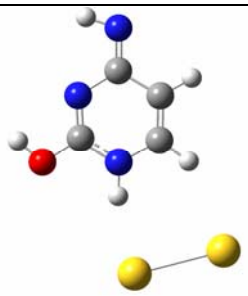
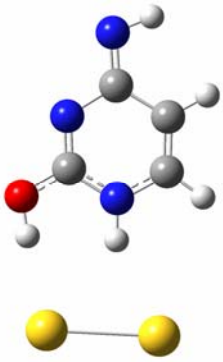
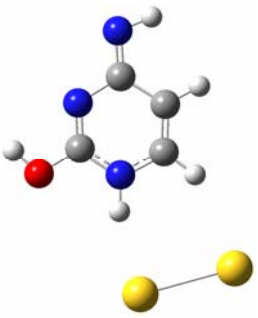
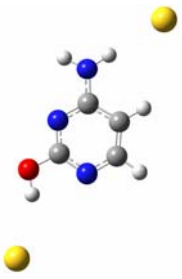
1.67			

*The energies are in eV.

Table S3 The optimized structures, VDEs, and ADEs of CAu_2^- for all the tautomers of cytosine*. The VDEs and ADEs were not calculated when the isomers are higher than the lowest-energy structure by more than 0.48 eV.

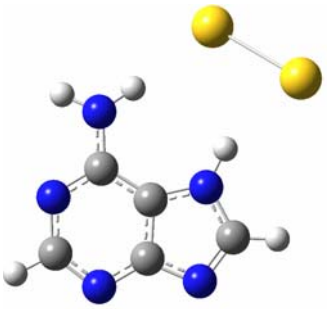
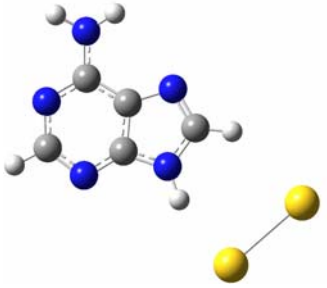
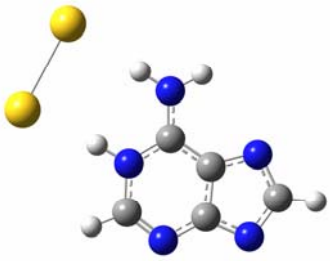
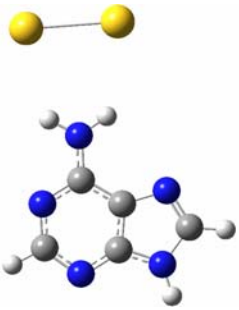
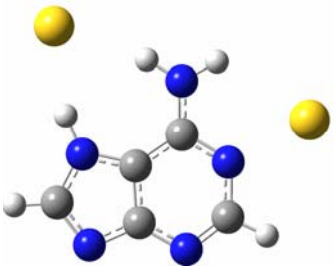
ΔE	Structures	VDE	ADE
0		2.84	2.67
0.06		3.03	2.13
0.07		2.84	2.13
0.09		2.74	1.83
0.14		2.75	2.57

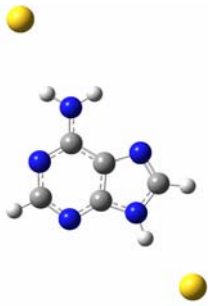
0.14		2.71	2.54
0.14		2.70	2.55
0.18		2.79	2.10
0.48			
0.60			

0.62			
0.76			
0.81			
0.88			
0.99		3.58	3.38

*The energies are in eV.

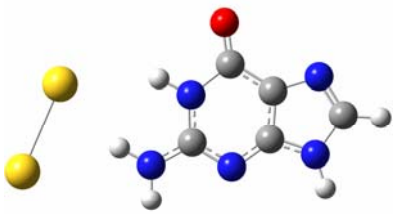
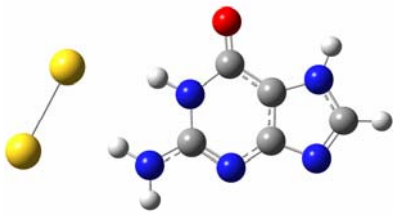
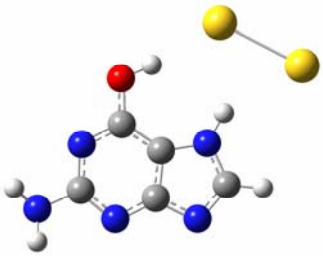
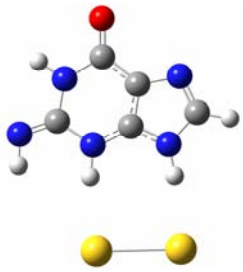
Table S4 The optimized structures, VDEs, and ADEs of AAu_2^- for all the tautomers of adenine*

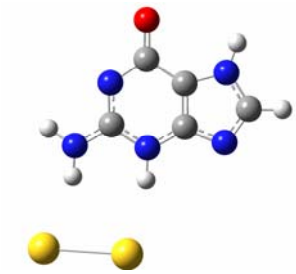
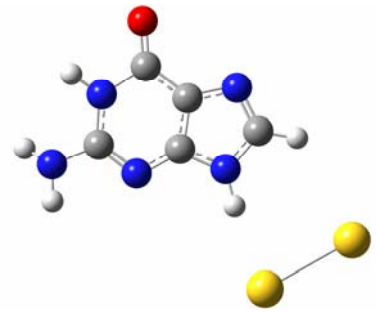
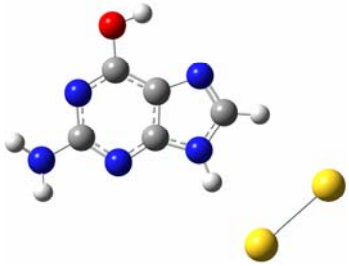
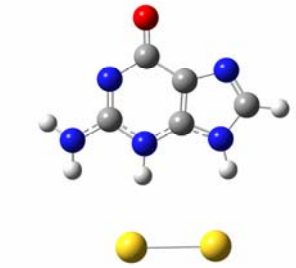
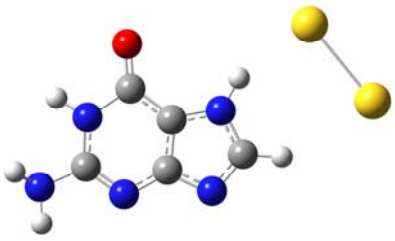
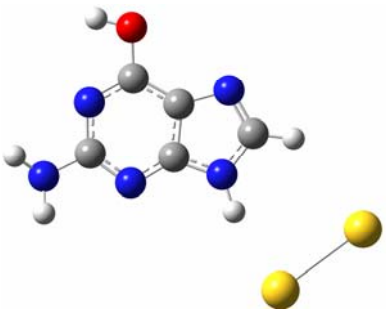
ΔE	Structures	VDE	ADE
0		3.15	2.94
0.11		2.75	2.57
0.22		3.40	3.18
0.40		2.48	2.34
0.64		3.79	3.64

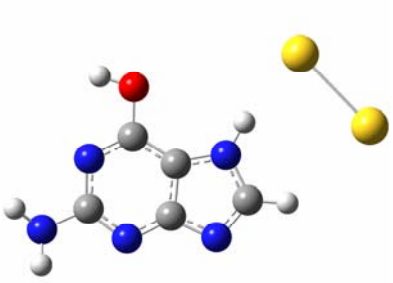
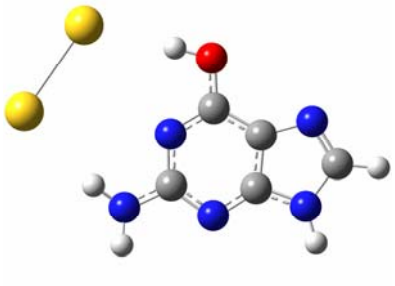
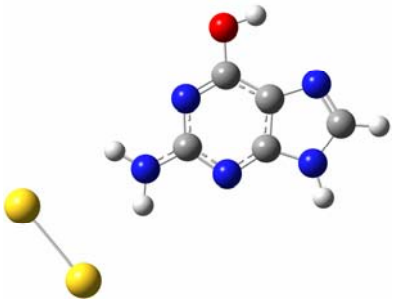
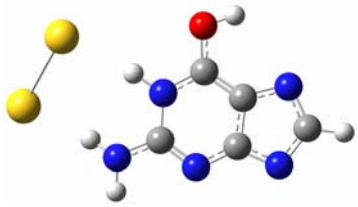
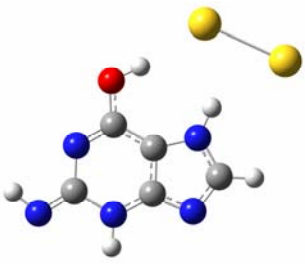
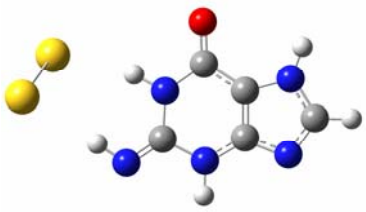
0.93		3.68	3.65

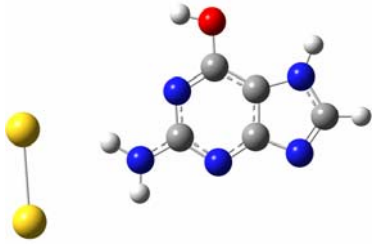
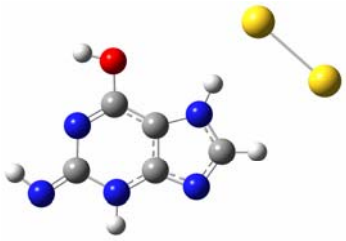
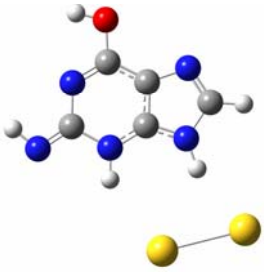
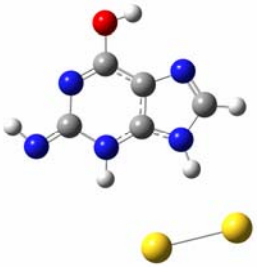
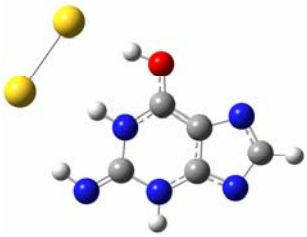
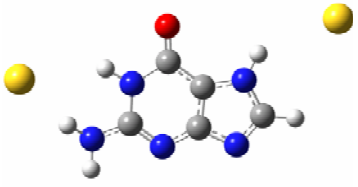
*The energies are in eV.

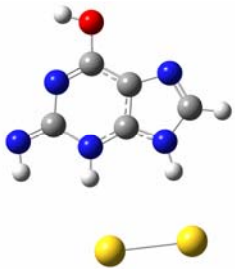
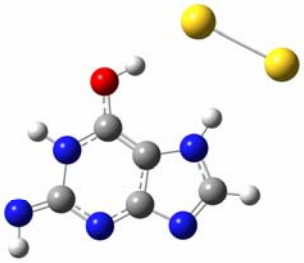
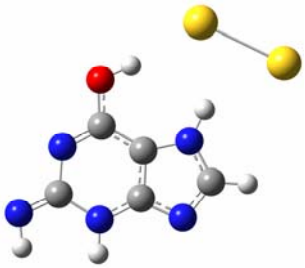
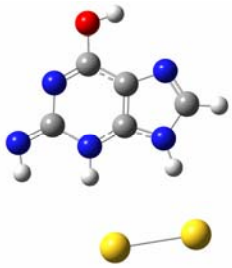
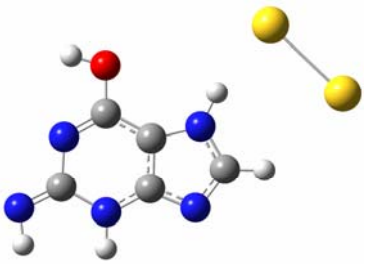
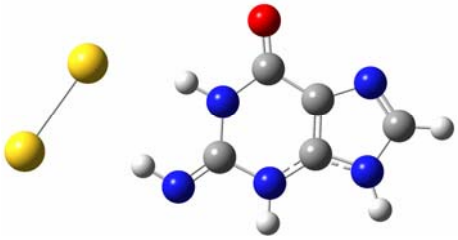
Table S5. The optimized structures, VDEs, and ADEs of GAu_2^- for all the tautomers of guanine*

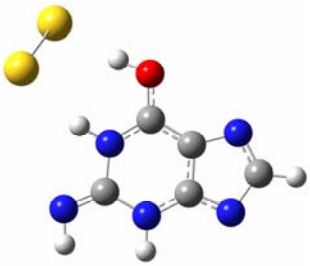
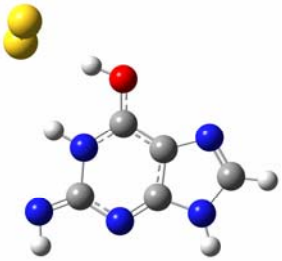
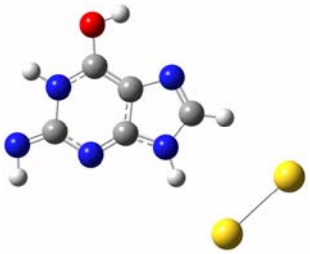
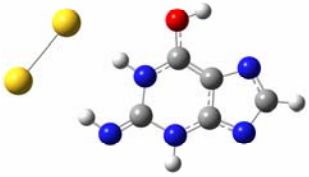
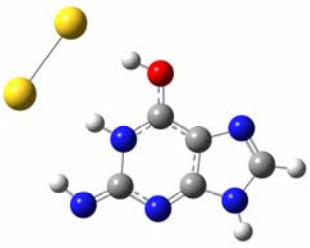
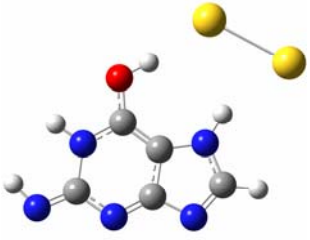
ΔE	Structures	VDE	ADE
0		2. 94	2. 09
0		2. 91	2. 70
0.1		3. 30	3. 02
0.15		3. 45	3. 28

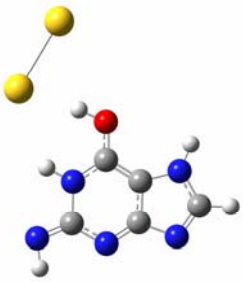
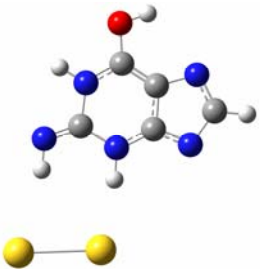
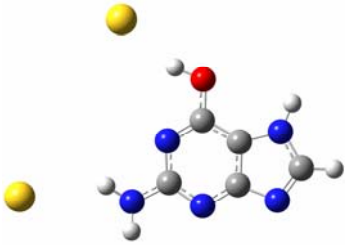
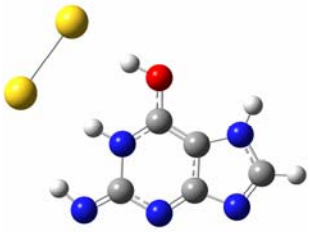
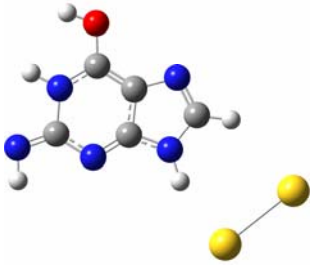
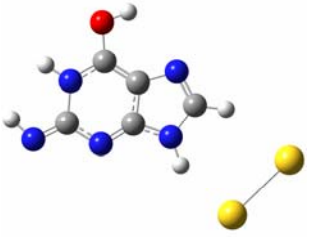
0.17		2.99	2.81
0.2		2.74	2.57
0.22		2.79	1.65
0.22		3.56	3.30
0.25		2.68	1.84
0.26		2.72	1.58

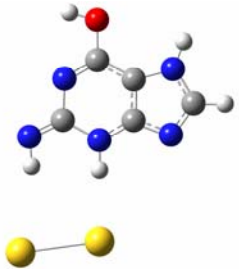
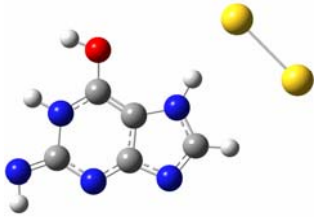
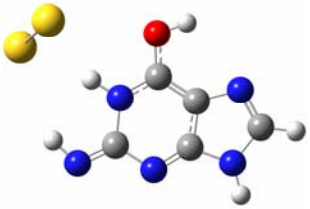
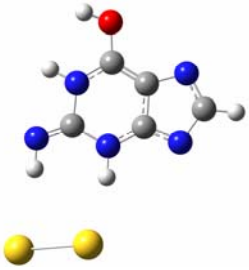
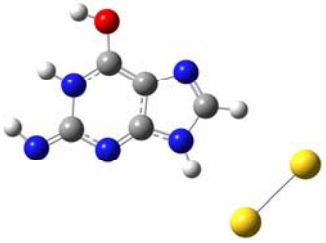
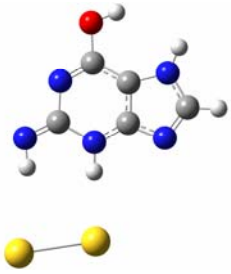
0.32		2. 77	2. 33
0.47		2. 62	2. 35
0.57		2. 48	2. 30
0.59			
0.62			
0.66			

0.67			
0.76			
0.77			
0.79			
0.80			
0.81			

0.85			
0.87			
0.91			
0.92			
1.00			
1.03			

1.05			
1.07			
1.09			
1.12			
1.12			
1.18			

1.23			
1.28			
1.33			
1.37			
1.41			
1.43			

1.49			
1.51			
1.55			
1.62			
1.79			
1.92			

*The energies are in eV.