Supporting Information

Computational Study of Transition States for Reaction Path of Energetic Material TKX-50

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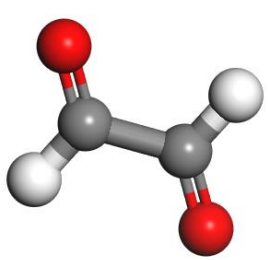
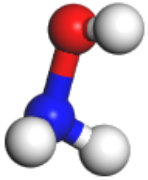
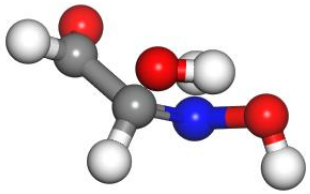
Figure S1. The geometries of the reactants, reaction complexes, transition states, product complexes, and products. N (blue), C (gray), H (white), O (red) and Cl (green)



1 [glyoxal]



NH_2OH



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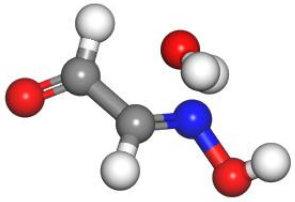

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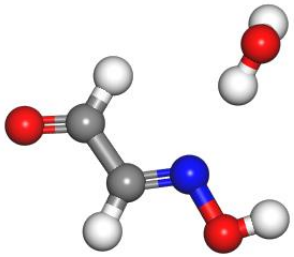

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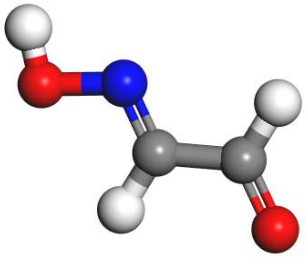

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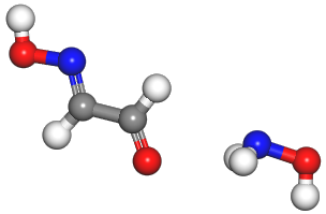

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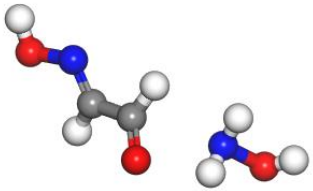

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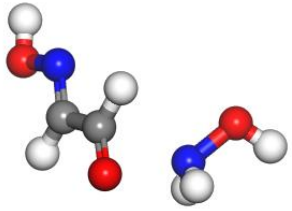

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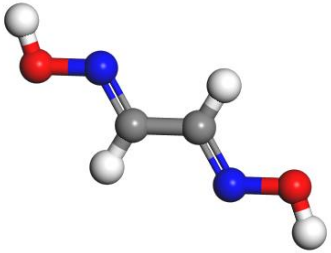

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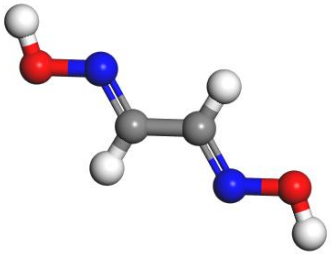

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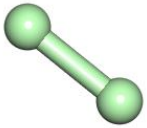

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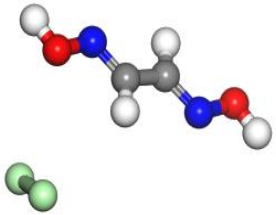

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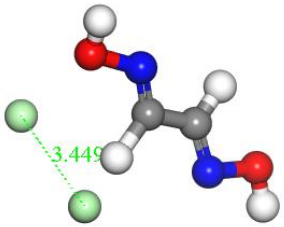

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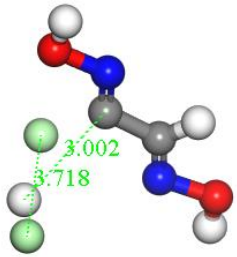

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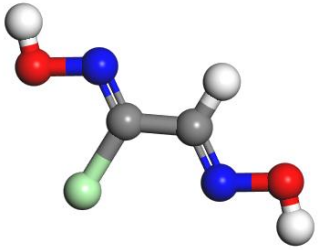

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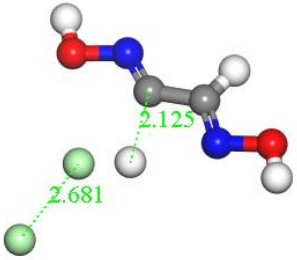

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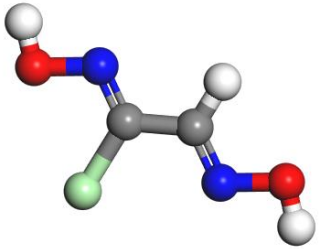

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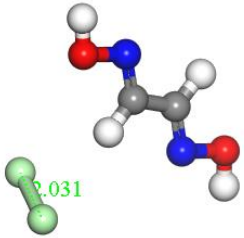

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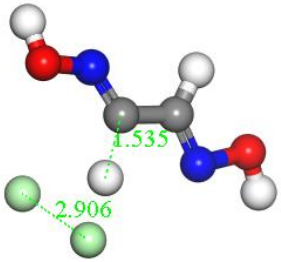

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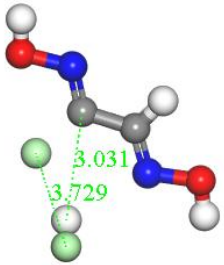

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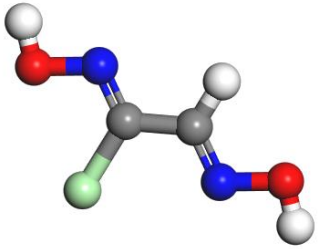

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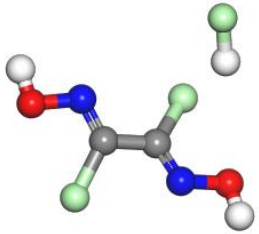

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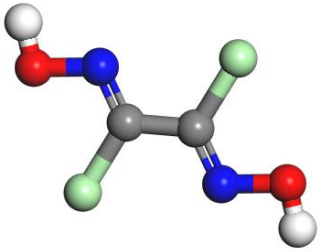
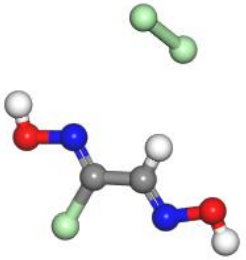


P6(3) [dichloroglyoxime]



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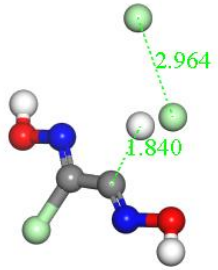

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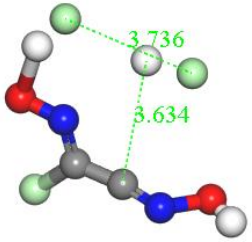

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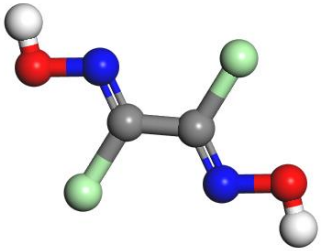

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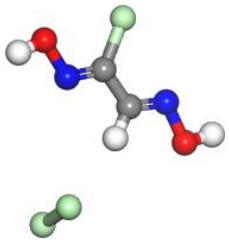

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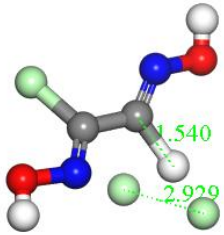

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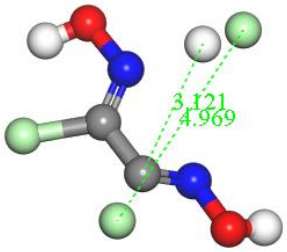

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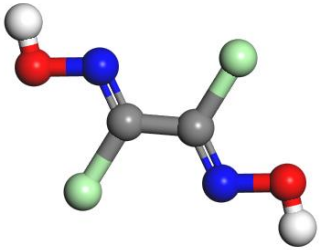

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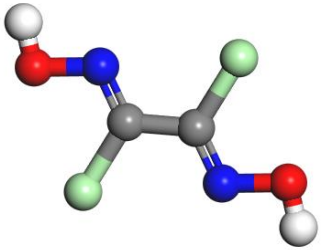

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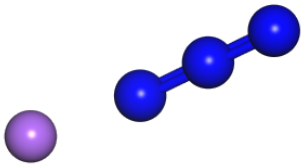

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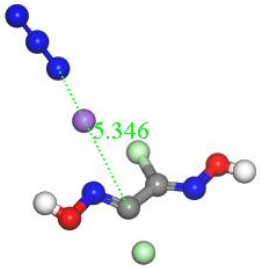

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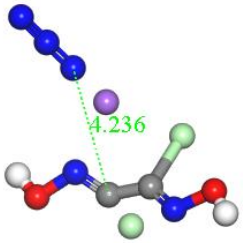

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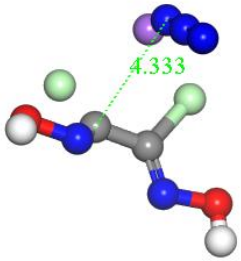

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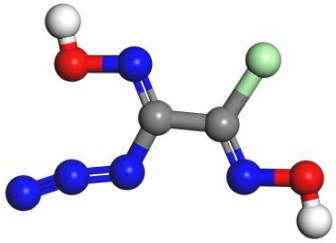

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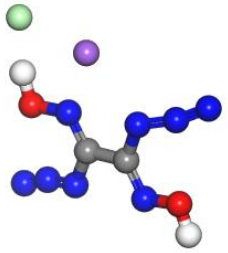

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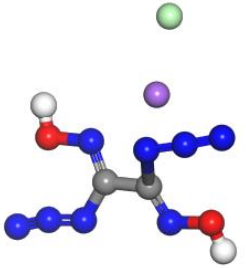

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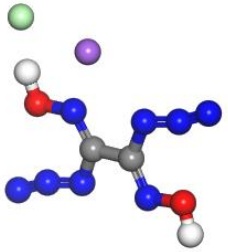

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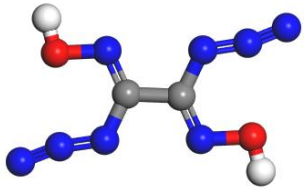

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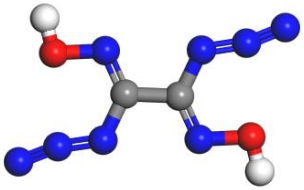

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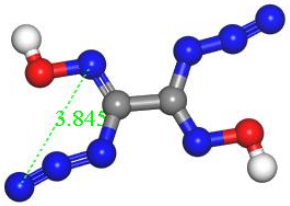

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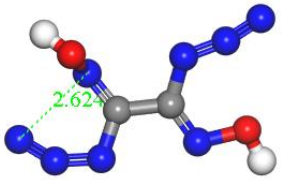

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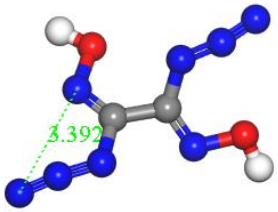

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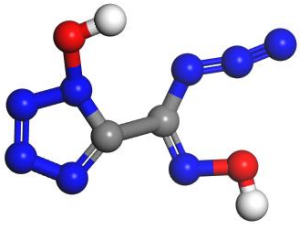

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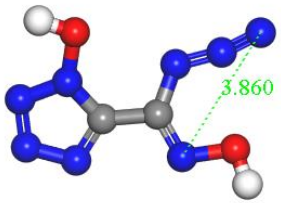

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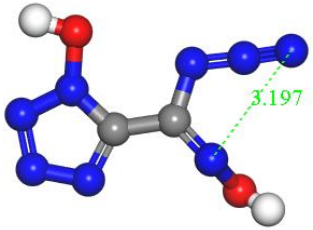

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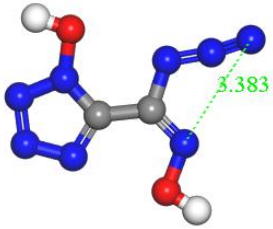

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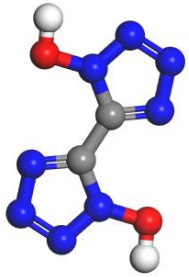

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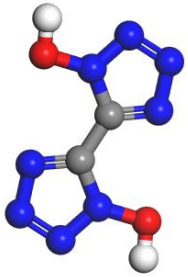

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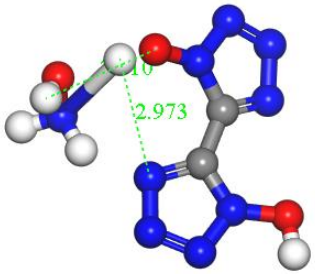

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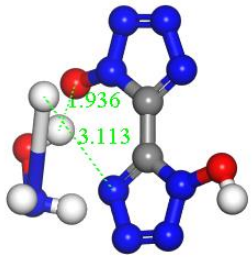

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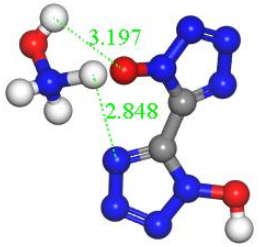

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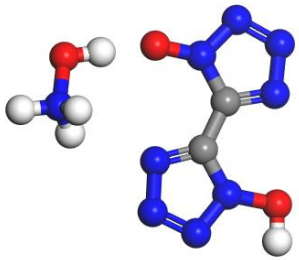
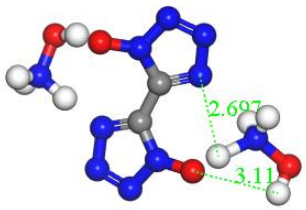
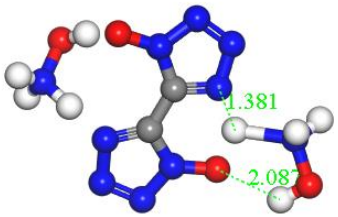


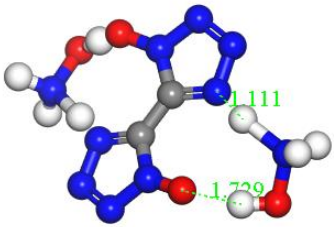
P13(5’)



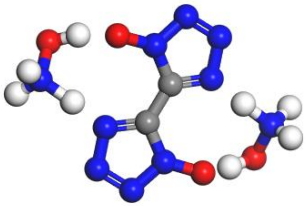
RC14



TS14



PC14



P14(6) [TKX-50]

Table S1. The structure properties of TKX-50 and $(C_2O_2N_8)^{2-}$ anion

	Atoms	Bond length（Å）		Atoms	Bond angle（degree）		Atoms	Dihedral angle（degree）	
		Initial	Optimized		Initial	Optimized		Initial	Optimized
TKX-50	H1-O1	0.996	0.998	O1-N1-H1	112.495	112.682	N5-C1-C2-N7	18.859	17.923
	O1-N1	1.444	1.440	N2-C1-C2	128.933	129.257	O2-N5-C1-C2	2.153	2.105
	N1-H1	1.598	1.594	N5-C1-C2	125.656	125.245			
	N2-C1	1.355	1.352	C1-N2-N3	109.300	109.243			
	C1-C2	1.422	1.421	C1-N5-O2	128.12	127.939			
	C1-N5	1.365	1.365						
	N5-O2	1.278	1.277						
	N3-N4	1.296	1.297						
$(C_2O_2N_8)^{2-}$	C1-C2	1.539	1.459	N1-C1-C2	125.967	125.848	N4-C1-C2-N5	30.000	85.275
	N1-C1	1.503	1.351	N4-C1-C2	125.772	125.664	O1-N4-C1-C2	-0.620	2.051
	N2-N3	1.493	1.333	C1-N4-O1	125.543	129.904			
	N4-C1	1.494	1.378	N3-N4-O1	125.831	122.952			
	N4-O1	1.480	1.293						

Table S2. The structure properties of other five molecules

	Atoms	Bond length（Å）		Atoms	Bond angle（°）		Atoms	Dihedral angle（°）	
		Initial	Optimized		Initial	Optimized		Initial	Optimized
glyoxal	O1-C1	1.512	1.220	O1-C1-H1	120.011	123.506	O1-C1-C2-O2	179.991	179.996
	H1-C1	1.140	1.115	O1-C1-C2	119.989	121.497	H1-C1-C2-H2	179.991	179.977
	C1-C2	1.537	1.521	H1-C1-C2	120.000	114.997			
glyoxime	H1-O1	1.110	0.975	H1-O1-N1	109.471	101.867	H1-O1-N1-C1	134.977	179.928
	O1-N1	1.481	1.406	O1-N1-C1	120.074	110.662	O1-N1-C1-C2	179.996	179.819
	N1-C1	1.506	1.294	N1-C1-C2	119.764	118.472	O1-N1-C1-H2	0.004	-0.166
	H2-C1	1.140	1.098	N1-C1-H2	120.236	122.257	N1-C1-C2-N2	179.997	179.998
	C1-C2	1.543	1.44	H2-C1-C2	120.000	119.271			
dichloroglyoxime	H1-O1	1.110	0.976	H1-O1-N1	109.471	101.487	H1-O1-N1-C1	128.391	179.899
	O1-N1	1.480	1.388	O1-N1-C1	119.991	113.793	O1-N1-C1-C2	177.031	179.908
	N1-C1	1.510	1.289	N1-C1-C2	120.012	119.174	O1-N1-C1-Cl1	-2.308	0.118
	Cl1-C1	1.559	1.468	N1-C1-Cl1	120.099	123.557	N1-C1-C2-N2	-177.628	179.915
	C1-C2	1.759	1.741	Cl1-C1-C2	119.885	117.268			
DAG	H1-O1	1.110	0.975	H1-O1-N1	117.061	101.857	H1-O1-N1-C1	-172.173	179.767
	O1-N1	1.496	1.402	O1-N1-C1	124.228	111.799	O1-N1-C1-C2	175.575	-179.183
	N1-C1	1.511	1.300	N1-C1-C2	119.921	116.632	O1-N1-C1-N2	-3.783	0.253
	C1-C2	1.542	1.481	N1-C1-N2	119.900	130.081	N1-C1-C2-N2	179.61	-179.899
	C1-N2	1.512	1.396	N2-C1-C2	119.921	113.348	C2-C1-N2-N3	-175.653	-174.425
	N2-N3	1.479	1.242	C1-N2-N3	119.972	123.581			
	N3-N4	1.482	1.145	N2-N3-N4	179.66	167.016			
1,1-BTO	H1-O1	1.110	0.984	H1-O1-N1	109.471	102.366	H1-O1-N1-C1	-172.464	178.486
	O1-N1	1.48	1.372	O1-N1-C1	125.406	128.112	H1-O1-N1-N2	7.516	-1.554
	N1-C1	1.469	1.355	N1-C1-C2	125.328	125.876	O1-N1-C1-C2	-0.012	0.048
	C4-C1	1.457	1.340	N1-C1-N4	108.955	106.491	O1-N1-C1-N4	179.994	179.855
	C1-C2	1.481	1.438	N4-C1-C2	125.717	127.633	N1-C1-C2-N5	-165.000	-179.602

N2-N3	1.491	1.314	O1-N1-N2	125.589	121.723

Table S3. The equilibrium constants of all reactions at different temperatures

T(K)	K_{eq}				
	glyoxal→glyoxime	glyoxime→dichloroglyoxime	dichloroglyoxime→DAG	DAG→1,1-BTO	1,1-BTO→TKX-50
250	0.124250228	11.25631837	0.000100091	0.027510504	1.68568×10^{-19}
275	0.101893329	5.963989976	0.000115342	0.032884190	2.27320×10^{-19}
298.15	0.088881672	3.703196266	0.000128310	0.037453528	2.84406×10^{-19}
300	0.087829040	3.584233742	0.000129378	0.037773728	2.88725×10^{-19}
325	0.079276058	2.358616057	0.000142801	0.041951810	3.52926×10^{-19}
350	0.073240152	1.657214422	0.000154074	0.045635737	4.16800×10^{-19}
375	0.069120155	1.236988039	0.000164783	0.048760867	4.80147×10^{-19}
400	0.066789218	0.967386671	0.000174104	0.051540566	5.44793×10^{-19}