

Supporting Information

An icosahedral cluster with spherical aromaticity

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Table S1. The Cartesian coordinate of optimized first seven isomers of Ta₁₂²⁺ cluster at B3P86/LANL2DZ level of theory.

Isomers	Cartesian coordinate			
A	Ta	0.00000000	0.00000000	2.53380119
	Ta	-2.15537930	-0.70032614	1.13315129
	Ta	2.15537930	-0.70032614	1.13315129
	Ta	1.33209767	-1.83347763	-1.13314786
	Ta	-1.33209767	-1.83347763	-1.13314786
	Ta	-0.00000000	0.00000000	-2.53380119
	Ta	-2.15538076	0.70032720	-1.13314786
	Ta	-1.33209711	1.83347592	1.13315129
	Ta	1.33209857	1.83347485	1.13315129
	Ta	2.15538167	0.70032442	-1.13314786
	Ta	0.00000146	2.26630193	-1.13314786
	Ta	0.00000090	-2.26630021	1.13315129
B	Ta	0.06728200	-2.64454800	-0.94679000
	Ta	2.32442100	-1.36885100	-0.76310300
	Ta	-2.11230600	-1.27478600	-1.59550200
	Ta	-1.89542000	1.28122200	-2.01365000
	Ta	0.19793600	0.21323400	-0.78554900
	Ta	0.94873300	-1.89455400	1.48673800
	Ta	2.30035900	0.28917900	1.29829800
	Ta	1.12699800	2.37917400	0.66431400
	Ta	-0.43037200	0.54742600	2.03608300
	Ta	-1.58413300	-1.77291800	1.01195400
	Ta	-2.76237900	0.43350000	0.38560200
	Ta	-1.30752700	2.55351900	0.22972900
C	Ta	-2.38358700	-1.23935800	1.48564200
	Ta	-2.38334800	1.23861700	1.48667200
	Ta	2.38448500	-1.23988400	1.48376900

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	Ta	2.38478700	1.23809100	1.48480500
	Ta	0.00033400	-0.00035100	0.85124300
	Ta	-1.28644600	-2.10981600	-0.72721600
	Ta	-2.69313400	0.00068900	-0.93077500
	Ta	-1.28598200	2.11072000	-0.72543300
	Ta	-0.00078400	0.00086000	-2.02115400
	Ta	1.28540200	-2.11010100	-0.72822300
	Ta	2.69239600	0.00009400	-0.93289100
	Ta	1.28587800	2.11043900	-0.72643700
D	Ta	1.25916500	1.51175800	1.40977500
	Ta	-1.42206800	1.42175900	1.02225700
	Ta	1.95236500	-1.36301600	1.86973600
	Ta	-2.52566500	-0.96779800	0.54629100
	Ta	-1.49032900	-1.92987100	-1.81857300
	Ta	0.34819700	1.88704800	-1.08450300
	Ta	-0.47745800	-0.51977600	2.66043900
	Ta	2.45418500	0.25462900	-0.56711600
	Ta	-1.98218800	0.59067500	-1.57387200
	Ta	0.47872700	-0.19184200	-2.59029700
	Ta	0.10512700	-0.89773500	0.04156400
	Ta	1.89814200	0.32227300	3.67620000
	Ta			
E	Ta	1.73158800	1.10913700	1.19931300
	Ta	-0.99286700	1.75397200	1.17424000
	Ta	0.79408500	-1.95337300	0.89947800
	Ta	-1.82243000	-0.95619500	0.90762200
	Ta	-0.67335900	-1.65376200	-1.32291900
	Ta	0.47190300	2.07818600	-0.95639900
	Ta	-0.17881100	-0.14765600	2.76106700
	Ta	1.81099800	-0.37055100	-1.18454300
	Ta	-2.07355800	0.80029300	-0.96093900
	Ta	-0.22752700	0.40890300	-2.74322800
	Ta	2.34161200	-0.93302000	2.89170200
	Ta	3.44666600	-1.06513200	0.77700600
	Ta			
F	Ta	0.16420500	-0.20680100	1.43696500
	Ta	-0.54021100	2.17925000	-0.09614100
	Ta	1.81771000	0.75621400	-0.63056800
	Ta	2.63737100	-1.48433500	0.88457100
	Ta	-1.63174200	-2.11766100	0.55759400
	Ta	-0.90323400	0.09901300	-1.45944900
	Ta	-2.40442400	0.34132500	1.02157700
	Ta	-3.42593800	-0.61687300	-1.12321600
	Ta	0.74695500	-1.89884000	-0.79759400
	Ta	-1.84644900	-2.38180200	-1.99415400
	Ta	1.24957600	2.33711800	1.62283200
	Ta			
	Ta			

	Ta	2.95428100	0.60769200	1.92628100
G	Ta	1.13869000	1.29480600	1.62439500
	Ta	-2.32817700	1.93236200	-0.75204700
	Ta	-0.20278400	0.10239900	-0.90804600
	Ta	-1.47395900	0.78765300	1.49736100
	Ta	0.11777200	2.69970600	-0.29988200
	Ta	1.99121000	-1.48934600	-1.33101400
	Ta	2.24051300	1.27739500	-1.16781200
	Ta	0.63374400	-1.45817300	1.41296100
	Ta	2.96011800	-0.26910300	0.69890300
	Ta	-2.83896800	-0.46621400	-0.87287200
	Ta	-0.35493400	-2.57703300	-0.93569300
	Ta	-1.88322600	-1.83445400	1.03374800

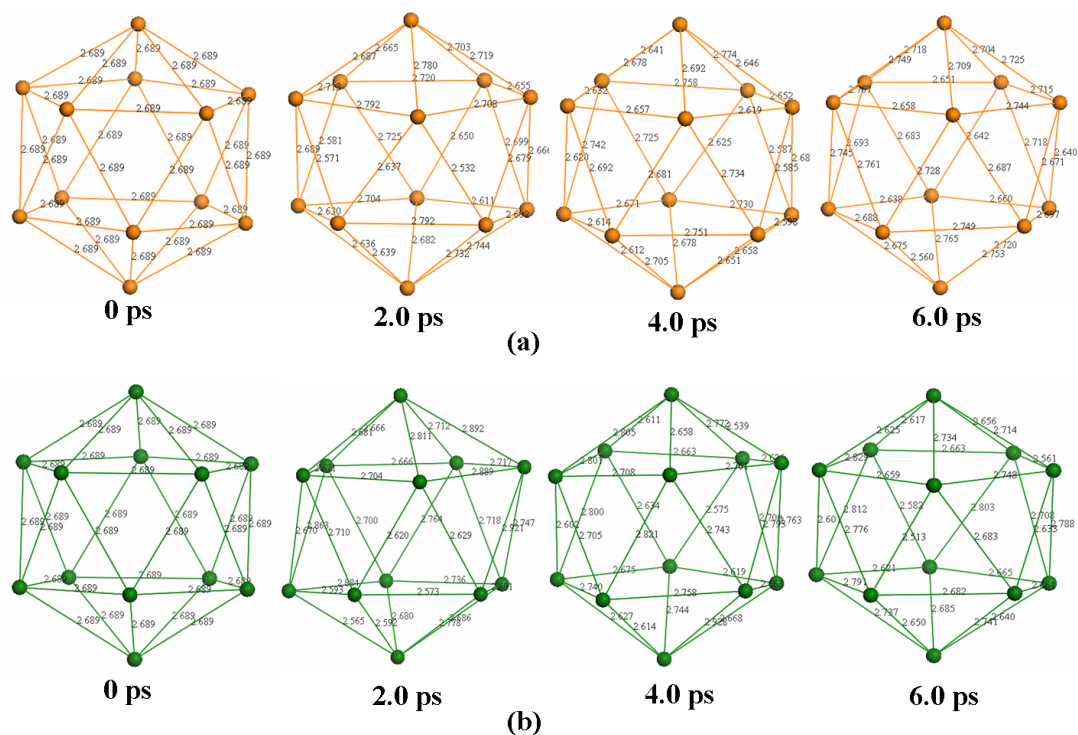


Figure S1. MD snapshots for icosahedral structure of Ta_{12}^{2+} cluster at different temperatures, (a). $T=300\text{K}$, (b). $T=600\text{K}$.