

Electronic Supporting Information: On the structure and electronic properties of Pt_n clusters: new most stable structures for $n=16-17^\dagger$

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Table 1 Theoretical and experimental bond lengths (d_{Pt-Pt}), vibrational frequency (ω), ionization potentials (IP) and dissociation energies (D_e) for Pt₂ dimer.

DFT functional	d_{Pt-Pt}	ω	IP	D_e
B3LYP	2.358	228.83	8.802	2.610
B3P86	2.335	238.34	8.978	2.758
PW91	2.353	227.07	9.028	4.010
B3PW91	2.336	237.81	8.846	2.682
BP86	2.354	225.93	9.095	3.668
BPW91	2.356	225.33	8.963	3.362
M06	2.365	223.23	8.997	2.939
M06-2X	2.306	253.14	8.409	1.534
M06-L	2.430	191.35	8.788	3.060
CAM-B3LYP	2.327	247.97	9.373	2.239
PBE0	2.328	241.72	8.710	2.608
TPSS	2.353	227.41	8.791	3.369
TPSSh	2.343	233.46	9.056	3.034
LC-BLYP	2.302	262.66	9.377	2.543
Exp. ^a	2.340	259.40	–	–
Exp. ^b	–	–	8.800	3.140

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^b Ref. (doi:9.1063/1.455577)

Cartesian coordinates

The lowest energy structures of Pt_n (n=15-17) clusters calculated using the Orca program and the TPSS/Def2TZVP approach.

Pt_{15_1}

Pt -3.58681344974439 -1.11065064262805 0.66992026141164
Pt -1.32435841953484 -2.13063450148272 1.18864612459464
Pt 0.99793905666440 -3.15504475688956 1.26958336504223
Pt -2.54949476624107 1.24156627537590 0.87928965937958
Pt -0.27477461484810 0.19424909843016 1.38252977179551
Pt 2.03478537953435 -0.86162361900176 1.51557950290291
Pt -1.16175028541180 3.19443619568735 -0.00644658272408
Pt 0.90648308735616 2.46683593674375 1.26428354852487
Pt 3.20908938856049 1.38980138157090 1.50493125967443
Pt -1.85077089188207 -0.21760593895605 -1.05117535887312
Pt -0.35235362785371 1.62334576961221 -1.86429642058122
Pt 0.31388419132917 -1.85438148004679 -0.82013784738236
Pt 1.67995344748687 0.82761398496138 -0.54143039794589
Pt -0.23218934433697 -0.64694948972005 -3.10310394922991
Pt 2.19037184892152 -0.96095821365665 -2.28817493658924

Pt_{15_2}

Pt -1.96200335395462 -1.20713663262998 -2.66138800582303
Pt -1.85671412026740 0.94795848122465 -1.29993620547597
Pt -1.82166799806916 3.02901413129850 0.16875951860604
Pt -2.03701919104700 -1.56642846744706 -0.13285766029248
Pt -1.99403270929692 0.82451878106190 1.47580198492387
Pt -2.07139525976386 -1.55394159353728 2.42500760983462
Pt 0.56643291418984 -1.32417507488435 -2.58559958880617
Pt 0.66862322121160 0.94767826922362 -1.46489707601335

Pt	0.72375130823661	2.89454666095117	0.13223642493761
Pt	0.45659359575909	-1.56709837705701	-0.09065733425622
Pt	0.49769512116928	0.72212831321755	1.40718802526883
Pt	0.47089729810347	-1.57053003370365	2.45056130570717
Pt	2.80008300181510	-0.65514264074895	-1.43818675919321
Pt	2.82741907263677	1.32422998039000	0.39918414605834
Pt	2.73133609927721	-1.24562179735909	1.21478461452395

Pt_{15_3}

Pt	-1.94676241973727	-1.08473600356136	-2.73219823413963
Pt	-1.77527186162463	0.60149514083752	-0.78780213927935
Pt	-1.78484115492614	3.03297250764613	0.04996484917108
Pt	-2.08877099732672	-1.84781816690541	-0.27924451294792
Pt	-1.94763197798445	1.04114385161928	1.68506608882830
Pt	-2.17584394251370	-1.44134954316053	2.25427319981957
Pt	0.58992626344741	-1.31465305245053	-2.61402351274041
Pt	0.70455973210382	0.92636817176937	-1.44282327197879
Pt	0.75308265286269	2.90783806827140	0.10061346478192
Pt	0.42405776489696	-1.66178687546090	-0.12760066660140
Pt	0.54836821642515	0.76174653807422	1.44611596596983
Pt	0.37475385023617	-1.55512192191056	2.41237742198179
Pt	2.83105605103661	-0.62775360962144	-1.47444685635731
Pt	2.86246996620201	1.41238790845654	0.33431762365143
Pt	2.63084685690208	-1.15073301360372	1.17541157984091

Pt_{16_1}

Pt	-2.94691437649493	-0.02126861436433	-1.36230067242425
Pt	1.61455907326112	-1.44061831808738	-2.70929453381246
Pt	1.47579206698029	-1.41917819821645	2.43170320366704
Pt	-0.48594060866457	1.12175776713598	-1.39486053757228
Pt	2.51199143597421	0.69048046647814	1.36381936002993
Pt	2.44263193443281	2.84192008935210	-0.03654264653053
Pt	2.01382904539281	0.76266151504195	-1.48862304506710
Pt	-0.89135415870206	-1.01063872670618	-2.67282412801297
Pt	-1.25074468060417	-1.55810265329453	2.37076001883812
Pt	0.27669733802017	-3.41953772686072	0.96004588065947
Pt	-0.00165338550138	0.66512490800281	1.54670302613498
Pt	-0.06316126324392	2.90458401371368	0.33156947913135
Pt	-2.51174390588872	2.49823030635441	-0.28731512992173
Pt	-2.52926872856945	0.43147615097174	1.30175301884008
Pt	-1.16401662424678	-1.58278765254186	-0.19968497282214
Pt	1.50929683775461	-1.46410332717941	-0.15490832113752

Pt_{16_2}

Pt	-2.19007104789273	-2.46020952030192	-1.89726072151274
Pt	-2.08300429354584	0.03676121030920	-1.24607959181531
Pt	-1.95611437277677	2.56980504694640	-1.74440273429894
Pt	-2.42993570467605	-1.73741396240237	0.54805381273326
Pt	-2.23042567542561	1.69426061145161	0.66305379509066
Pt	-2.65155860816597	-0.07220857614812	2.45856256896741
Pt	0.38063086403603	-2.62118331716828	-1.50303709729825

Pt	0.48664938751694	-0.065541944445977	-1.60048379372071
Pt	0.57536548381291	2.45464592913171	-1.42368894234646
Pt	0.10137552006882	-1.61142030356910	0.78042578948666
Pt	0.26174231673160	1.38706330920154	0.87819640250305
Pt	-0.08837066563982	-0.16977474329662	2.85428007322457
Pt	2.49723121435097	-1.35366474007832	-0.65573260865228
Pt	2.67015548919352	1.95618261200190	-0.07380004767295
Pt	2.24842539957492	-0.15329517977366	1.74516551493259
Pt	4.40790469303711	0.14599356815579	0.21674758017945

Pt_{16_3}

Pt	2.40987208266111	-1.97559492594514	-2.13877092071682
Pt	2.25740966391010	-1.64674528351881	0.37443127090371
Pt	2.14792849253343	-0.85889377283214	2.80586250660743
Pt	2.26848918577175	0.47755219990839	-1.54404857294710
Pt	2.20608298754611	1.05675620825423	1.12337643476817
Pt	2.23830184038499	2.86552922648455	-0.69106203861214
Pt	-0.20393046270393	-1.98763561531273	-2.22309054340737
Pt	-0.25995498223341	-1.61797808768486	0.26423841427745
Pt	-0.39082174404952	-0.83995303447344	2.70315724682470
Pt	-0.28267730012269	0.49064727596044	-1.65932706433640
Pt	-0.31388986239117	1.12021168343777	1.09465508394156
Pt	-0.32269051064674	2.85767445192787	-0.79767442818181
Pt	-2.42481915286648	-0.96922364801071	-1.28269746292602
Pt	-2.58079021091854	-1.25433555274334	1.44702904242465
Pt	-2.51424709410976	2.06120587958832	0.29411933776093
Pt	-4.23426293286526	0.22078299495959	0.22980169371905

Pt_{17_1}

Pt	-1.74785205534511	-3.27409201997187	0.00013765566559
Pt	-2.19454363524043	-1.18667117747465	1.38658216798780
Pt	-2.61713704586646	1.04654871861378	2.54897407390122
Pt	0.74787135946442	-2.85070532028757	0.00000435917382
Pt	3.24467326279591	-2.41664579666271	0.00000844348542
Pt	0.29631197026039	-0.70408538678237	1.34691046781771
Pt	-0.12549784015134	1.54313247818205	2.49929994019598
Pt	2.76718034235212	-0.20653923153848	1.26030030173454
Pt	2.10559965113622	2.24733187592982	1.40232279534396
Pt	-2.19428220795922	-1.18623357991033	-1.38560100253840
Pt	-2.57070588775124	1.19638344260928	0.00072223031716
Pt	-2.61898821439605	1.04675174531272	-2.54752878915908
Pt	0.29703751332421	-0.70421026868584	-1.34749805200048
Pt	-0.13484502050766	1.86532758777002	-0.00028906221193
Pt	-0.12735546971035	1.54278594864968	-2.49970732699485
Pt	2.76770684618256	-0.20607866991896	-1.25973253741154
Pt	2.10482543141203	2.24699965416541	-1.40490766530693

Pt_{17_2}

Pt	-1.30071590570662	-2.98114350507865	-0.01454861720070
Pt	-2.50720582976098	-0.66696851755488	0.76664309282224
Pt	-2.42594073280159	1.16933609613103	2.60220670877155

Pt	1.33197344080755	-2.80729462950293	-0.55976859327860
Pt	2.46902121554166	-1.26019475566966	1.21870904462755
Pt	-0.02263828028062	-0.98439630108746	1.13064601342871
Pt	0.10519730537173	1.18674180156457	2.45282000211119
Pt	2.63379072825299	1.08834459457835	2.23970438984568
Pt	2.29919289068333	1.71344304694731	-2.70598557576806
Pt	2.61807026687983	-0.37317830631013	-1.17471067970627
Pt	-2.30491017831860	-1.24922373818352	-1.68897705913488
Pt	-2.60893772864597	1.77451177336755	0.10137819272096
Pt	-2.73969220912710	1.19297519525539	-2.37526528471574
Pt	0.14390447082935	-0.72090991009144	-1.55925636642534
Pt	-0.08516770137822	1.72087677586497	-0.03654503549101
Pt	2.42699834257468	1.94196147806492	-0.14874632060733
Pt	-0.23463992412144	1.58571000790457	-2.57929054279993

Pt_{17_3}

Pt	-2.09039544866261	-3.16139231547537	-0.20036619187338
Pt	-2.05671246855048	-1.37658449663417	1.65669414070448
Pt	-2.20848461840247	1.00928947379408	2.55538136010064
Pt	0.44080407247511	-2.94109796777134	-0.23923128542637
Pt	2.66326755530333	-1.97565786930141	0.58275309795481
Pt	0.43333612847638	-0.95239838448088	1.33896087710281
Pt	0.29331071166780	1.32180297792209	2.48443942722977
Pt	2.52509467964575	2.36307773823051	2.39074915944205
Pt	2.44998078799805	1.91328581488883	-2.63787214669898
Pt	2.59781027045204	-0.16568156159121	-1.15741997039358
Pt	-2.30634634196972	-1.20982367227317	-1.82972738786542
Pt	-2.29143592759291	0.50502175115033	0.01144767177130
Pt	-2.54787002205858	1.28184747365951	-2.43684152553441
Pt	0.19028792440000	-0.77975647299535	-1.57202681144546
Pt	0.04735316347527	1.60662948586343	-0.01840409914385
Pt	2.48624104360696	2.19140479809879	-0.08337143107568
Pt	-0.04588151026394	1.57095522691534	-2.56844188484871