Electronic Supplementary Information for Dalton Transactions

Polyhedral Structures with an Odd Number of Vertices: Nine-Atom Clusters and Supramolecular Architectures.

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Electronic Supplementary Information

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Table S1. Atomic Coordinates for Ideal 9-vertex Polyhedra

SG-9 (square grid)

Tr1	-1.0	1.0	0.0
Tr2	0.0	1.0	0.0
Tr3	1.0	1.0	0.0
Tr4	-1.0	0.0	0.0
Tr5	0.0	0.0	0.0
Tr6	1.0	0.0	0.0
Tr7	-1.0	-1.0	0.0
Tr8	-1.0	-1.0	0.0
Tr9	1.0	-1.0	0.0

L-9 (linear chain)

Tr1	-4.0	0.0	0.0
Tr2	-3.0	0.0	0.0
Tr3	-2.0	0.0	0.0
Tr4	-1.0	0.0	0.0
Tr5	0.0	0.0	0.0
Tr6	1.0	0.0	0.0
Tr7	2.0	0.0	0.0
Tr8	3.0	0.0	0.0
Tr9	4.0	0.0	0.0

HG-9 (hexagonal grid)

Tr1	0.0	1.0	0.0
Tr2	-0.866	0.5	0.0
Tr3	0.866	0.5	0.0
Tr4	-1.732	0.0	0.0
Tr5	0.0	0.0	0.0
Tr6	1.732	0.0	0.0
Tr7	-0.866	-0.5	0.0
Tr8	0.866	-0.5	0.0
Tr9	0.0	-1.0	0.0

Table S2. Shape Measure of Some Transition Metal Clusters Relative to their Closest Ideal Shape (supplements the information of Table 2).

Refcode	M_9	Shape	S(shape)
JUTFIN	Ni_9	4:5	2.63
JUTDUX	Ni_9	4:5	2.65
DOMMAT	Ni_9	4:5	2.88
JUTFAF	Ni_9	4:5	2.90
KAQTUR	Co_9	cCU-8	0.00
VEDZOT	Pd_9	cCU-8	0.00
SIWJUD	Pd_9	cCU-8	0.00
LETWEM	Co_9	cCU-8	0.07
LETWEM01	Co_9	cCU-8	0.07
SAKTUT	Ag_9	cCU-8	1.81
SIWJOX	Pd_9	cCU-8	4.33
AGEVIR	Ni_9	CP-9	0.21
GUNTUE	Ni_6Rh_3	CP-9	0.25
CESCIM	Ag_6Fe_3	CP-9	0.79
CAVKIT	Os_9	CP-9	3.67
CAVKEP	Os_9	CP-9	3.77
JAPWOM	Au_8Rh	cvIC-8	0.38
JAPWOM10	Au_8Rh	cvIC-8	0.38
SIYWIG	Au_8Pd	cvIC-8	0.48
ROQTOG	Au_8Pt	cvIC-8	0.50
JABMUU	Au_9Pt	cvIC-8	0.95
JOVGOQ	Re_9	fOC-9	0.02
CAQPUF	Rh_9	fOC-9	0.03
DOXKAC	Rh_8Pt	fOC-9	0.03
CEDSIO	Rh_8Ni	fOC-9	0.06
WETVUM	Ir_9	fOC-9	0.07
VIPJIN	Ir_9	fOC-9	0.08
FANBAX	Co_9	fOC-9	0.13
PONGOO	Ru_6Pt	fOC-9	0.20
NAMDIO	Ru_6Pt_3	fOC-9	0.23
PONGUU	Ru_6Pt_3	fOC-9	0.23
NAMGUD	Ru_6Pt_3	fOC-9	0.29
JUTBEF	Ru_6Pt_3	fOC-9	0.30
JUTBEF10	Ru_6Pt_3	fOC-9	0.30
JUTBIJ10	Ru_6Pt_3	fOC-9	0.32
JUTBIJ	Ru_6Pt_3	fOC-9	0.32

SSEPNI	Ni_9	fOC-9	0.35
SSEPNI10	Ni_9	fOC-9	0.36
POCLEY	Ru_6Pt_3	fOC-9	0.36
HABKUQ	Ru_6Pt_3	fOC-9	0.36
GISZOX	Co_9	fOC-9	1.54
FALGUU	Ni_9	fOC-9	4.29
DILRUL	Cu_5Fe_4	HG-9	0.13
YEMXAP	Ag_5Fe_4	HG-9	0.22
HENSOI	Ru_9	JCCU-9	3.64
CURPAG	Ni_9	JGSP-9	0.08
BEAMRH	Rh_9	JGSP-9	0.09
XALNED	Ni_9	L-9	0.01
XALNED	Ni_9	L-9	0.01
CONTII	Co_9	rCSAPR-9	0.33
JUXLUJ	Ru_5Co_4	rTCTPR-9	4.41
BETROH	Au_9	c-SAPR-8	0.74
CEGVIT	Au_9	c-SAPR-8	0.75
VAPYIU	Au_8Pd	c-SAPR-8	1.26
PHTPTC	Pt_9	TCL-9	1.59
VAZWUO	Au_7Co_2	vTRPY-9	0.21
RAXPUC	Au_7Re_2	vTRPY-9	0.95

Table S3. Shape Measures for Clusters of Group 13 and 14 Elements (data corresponding to Figure 4).

Refcode	M_9	S(CSAPR)	S(TCTPR)	Dev.*
18 framework electrons:				
B_9Cl_9	B_9	1.54	1.04	0.54
OHILUM	Ga_9	1.58	0.42	0.30
84956	B_9	1.48	0.81	0.44
410698	B_9	1.49	0.74	0.42
19 framework electrons:				
GOXWUL	B_9	1.67	0.53	0.38
20 framework electrons:				
BIFWOC	$TlSn_8$			
MDCCNB	B_7C_2	2.44	1.30	0.84
MDCCNB	B_7C_2	2.39	1.27	0.82
GOXXAS	B_9	2.27	0.89	0.67
21 framework electrons:				
BEHMOR	Ge_9	0.71	2.07	0.56
CAJBEU	Sn_9	1.50	0.46	0.30
CUFSIF	Ge_9	0.60	0.98	0.20
DALHIH	Sn_9	0.33	2.19	0.40
HOQQUZ	Ge_9	0.66	0.93	0.21
HOQQUZ	Ge_9	0.37	1.56	0.27
HOQRAG	Ge_9	0.58	1.19	0.26
HOQRAG	Ge_9	0.34	2.03	0.37
NECPIV	Ge_9	0.61	1.77	0.44
NECPOB	Ge_9	0.80	0.97	0.28
NECPUH	Ge_9	0.54	1.35	0.29
SOGGAW	Ge_9	1.24	1.65	0.63
SOGGAW10	Ge_9	1.24	1.65	0.63
XAGDEO	Sn_9	0.84	0.65	0.17
XAGDEO01	Sn_9	1.29	0.42	0.22
YENBIC	Pb_9	1.06	0.58	0.22
YENBIF10	Sn_9	0.97	0.62	0.21
YENBIF10	Sn_9	0.76	1.32	0.38
YENBOI	Ge_9	1.05	1.78	0.61
YENBOI01	Ge_9	1.05	1.78	0.61
ZIMTAQ	Pb_9	1.05	0.57	0.21
22 framework electrons:				
BEHLOQ	Ge_9	0.84	0.85	0.25
BEHLUW	Ge_9	0.88	0.58	0.16

BEHLUW	Ge_9	0.90	0.57	0.16
BEHLUW	Ge_9	0.79	0.67	0.16
BEHMAD	Ge_9	0.54	1.39	0.30
BEHMIL	Ge_9	1.37	1.39	0.60
26227	Bi_9	1.63	1.35	0.66
CRNASN01	Sn_9	0.37	2.41	0.47
CRYGER	Ge_9	0.80	0.96	0.28
CRYGER	Ge_9	0.42	2.28	0.47
Cs_4Ge_9	Ge_9	0.39	2.18	0.43
ENNASN10	Sn_9	1.30	2.11	0.77
EQULIL	Ge_9	0.35	1.75	0.31
EQULOR	Ge_9	0.48	1.55	0.32
EQULOR	Ge_9	0.52	1.57	0.35
EQULUX	Ge_9	0.50	1.28	0.25
EQULUX	Ge_9	0.59	1.26	0.29
EQUMAE	Ge_9	0.36	1.59	0.27
EQUMAE	Ge_9	0.38	1.79	0.33
FAFPAE	Ge_9	1.02	0.49	0.16
FAFPEI	Ge_9	0.95	0.54	0.16
GUDJAQ	Ge_9	0.46	1.67	0.34
K_4Sn_9	Sn_9	0.34	2.29	0.43
KAWXUC	Ge_9	0.64	0.79	0.15
Li_4Sn_9	Sn_9	0.31	2.22	0.39
OHOHEY	Ge_9	2.74	3.96	1.49
PUPGEM	Ge_9	0.76	1.66	0.47
PUPGEM	Ge_9	0.74	1.80	0.50
PUPGEM	Ge_9	0.44	2.51	0.53
Rb_4Pb_9	Pb_9	0.59	2.63	0.63
SUYTIP	Ge_9	0.67	1.47	0.38
VARPEK	Sn_9	0.92	1.27	0.42
VODTAJ	Sn_9	0.31	2.30	0.41
XAGPEB	Ge_9	0.92	0.58	0.17
XAGPIF	Ge_9	0.88	0.69	0.20
XAGPIF	Ge_9	0.85	0.65	0.18
XAGPOL	Ge_9	0.83	0.82	0.23
XAGQAY	Ge_9	1.20	1.28	0.52
XAGQEC	Ge_9	0.80	1.01	0.29
XAGQIG	Ge_9	0.86	0.70	0.20
XAGQOM	Ge_9	1.01	0.54	0.19
XAGQOM	Ge_9	0.96	0.60	0.19

XUGTOI	Ge_9	1.12	0.71	0.30
XUGTOI	Ge_9	1.19	0.71	0.31
XUGTOI	Ge_9	1.22	0.72	0.33
ZIMSUJ	Pb_9	0.37	2.35	0.46
24 framework electrons:				
MCNBOR	B_7C_2	9.63	7.22	2.99
B_9H_{15}	B_9	13.19	14.28	4.16
CsB_9H_{14}	B_9	10.90	8.35	3.28

* Value of the deviation function from the minimal interconversion path.

Table S4. Shape measures of Supramolecular Assemblies with nine transition metal atoms relative to their closest ideal shape.

Refcode	M_9	Shape	S(shape)
JEBSEO	Ni_9	cCU-8	0.00
IBEZIY	Co_9	cCU-8	0.82
JAXSOQ	Co_9	cCU-8	0.92
ACOFON	Ni_9	cCU-8	0.94
BEQYUS	Fe_9	cCU-8	0.94
BEQYUS	Fe_9	cCU-8	1.22
ACOFIH	Ni_9	cCU-8	1.26
EVADOU	Sm_9	cSAP-8	0.01
EVADOU	Sm_9	cSAP-8	0.01
PECFEJ	Sm_9	cSAP-8	0.01
RAKPID	Eu_9	cSAP-8	0.01
HOVDAX	Y_9	cSAP-8	0.02
CUNDOE10	$Fe_7$2Mo	dT-9	0.15
CUNDOE20	$Fe_7$2Mo	dT-9	0.15
TBBZFM10	Cu_9	dT-9	0.22
BAESMC	$Fe_7$2W	dT-9	0.22
JASCIP	Fe_7Re	dT-9	0.24
JASCIP10	Fe_7Re	dT-9	0.24
JETBAL	Fe_7Re	dT-9	0.24
BMETFM10	$Fe_7$2Mo	dT-9	0.31
VOMKUD	Cu_9	dT-9	0.35
KARFIT	Ni_9	dT-9	0.99
KARFIT	Ni_9	dT-9	1.06
ZOPBOV	Au_8Pd	dT-9	2.98
ZOPBOV10	Au_8Pd	dT-9	2.98
UGUTEV	Co_9	dT-9	3.40
CATMAM	Cr_8Cd	EP-9	0.34
AHAYOX01	Ni_9	EP-9	0.76
QOZPIE	Pd_6Zn_3	fOC-9	0.38
GIWKIG	Cu_9	fOC-9	4.12
JOZCAC	Cd_9	HG-9	0.06
YESYIE	Ir_8Fe	HG-9	1.35
ECAQOP	Fe_9	HG-9	2.00
WIHBAQ	Cu_9	JCCU-9	0.07
ZUBKEM	W_9	JTC-9	0.14
EGIQUG	Mn_9	JTC-9	4.41

DERPEV	Cu_9	JTTP-9	0.43
GUCVAB	Ni_9	rTCTPR-9	0.49
EBAKAU	Mn_9	SG-9	0.47
MURMUH	Mn_9	SG-9	0.77
EBAKIC	Mn_9	SG-9	0.81
FAJJOQ	Mn_9	SG-9	0.84
SURDIS	Co_9	SG-9	1.29
MURNAO	Mn_9	SG-9	1.51
EBAKUO	Mn_9	SG-9	1.72
EBAKEY	Mn_9	SG-9	2.02
WONSOH	Au_6Fe_3	SG-9	2.09
EBAKOI	Mn_9	SG-9	2.15
FAJKEH	Mn_9	SG-9	2.28
FAJKEH01	Mn_9	SG-9	2.45
EBAKIC	Mn_9	SG-9	2.48
FAPGUZ	Cu_9	SG-9	2.56
MURNES	Zn_9	SG-9	2.65
KANBOQ	Mn_9	SG-9	2.75
FAJKAD	Mn_9	SG-9	2.81
AGOYEA	Cu_9	SG-9	2.82
FAJJUW	Mn_9	SG-9	3.05
EBALAV	Mn_9	SG-9	3.97
ROJFUR	Co_9	vTBPY-9	0.20

Table S5. Shape Measures and Path Deviation Functions for Supramolecular Assemblies forming 3x3 Grids (Figure 7).

Refcode	S(SG-9)	S(HL-9)	Dev. (%)
EBAKAU (**c**)	0.47	6.69	26
MURMUH	0.77	5.29	22
EBAKIC	0.81	5.67	74
FAJJOQ	0.84	5.69	27
SURDIS	1.29	7.83	52
MURNAO	1.51	3.80	22
EBAKUO	1.72	3.07	18
EBAKEY	2.02	8.59	68
WONSOH	2.09	8.54	69
EBAKOI	2.15	8.44	69
FAJKEH	2.28	8.08	68
FAJKEH01	2.45	8.32	72
EBAKIC	2.48	8.60	26
YESYIE (**b**)	2.52	1.35	5
FAPGUZ	2.56	7.74	69
MURNES	2.65	9.15	80
KANBOQ	2.75	9.14	81
FAJKAD	2.81	9.26	82
AGOYEA	2.82	7.27	69
FAJJUW	3.05	9.54	87
EBALAV	3.97	10.41	102
YEMXAP (**d**)	5.25	0.22	6
DILRUL (**d**)	5.49	0.13	4
NEPFAP	5.62	11.77	125
JOZCAC (**a**)	6.70	0.06	9
ECAQOP	8.50	2.00	67