10.1071/CH19557_AC

Australian Journal of Chemistry 2020, 73(8), 767-774

Supplementary Material

A Detailed Classification of Three-Centre-Two-Electron Bonds

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Table S1a. Coordinates of the optimised geometry of B_2H_6

B_2H_6	atomic no.	x	y	z
MP2/6-311++G(d,p)	5	0.884983000	-0.000001000	0.000016000
	1	1.456492000	-1.040890000	0.000783000
	1	-0.000060000	-0.002048000	-0.975257000
	1	1.455587000	1.041402000	-0.000843000
	5	-0.884975000	-0.000011000	-0.000023000
	1	-1.456210000	-1.041067000	0.000844000
	1	-0.000038000	0.001412000	0.975277000
	1	-1.455811000	1.041250000	-0.000770000
B3LYP/ aug-cc-pVTZ	5	0.879060000	0.000002000	0.000000000
	1	1.456440000	-1.035011000	0.000165000
	1	0.000002000	-0.000482000	-0.973617000
	1	1.456195000	1.035150000	-0.000164000
	5	-0.879060000	0.000001000	0.000001000
	1	-1.456421000	-1.035024000	0.000166000
	1	0.000003000	0.000221000	0.973610000
	1	-1.456219000	1.035135000	-0.000166000

Table S1b. Coordinates of the optimised geometry of CH_5^+

CH_5^+	atomic no.	x	y	z
MP2/6-311++G(d,p)	6	-0.117225000	-0.010424000	0.000029000
	1	-0.522944000	-0.374575000	-0.942459000
	1	-0.165147000	1.099610000	-0.000620000
	1	-0.522646000	-0.373640000	0.942993000
	1	1.018554000	0.339584000	-0.000053000
	1	0.895533000	-0.628433000	-0.000033000
B3LYP/ aug-cc-pVTZ	6	-0.111686000	-0.015102000	-0.000018000
	1	-0.506616000	-0.394768000	-0.939702000
	1	0.915281000	-0.598295000	-0.000080000
	1	-0.233975000	1.087875000	0.000496000
	1	-0.506303000	-0.395374000	0.939574000
	1	1.001729000	0.391172000	-0.000181000

Table S1c. Coordinates of the optimised geometry of CH_3-$C_2H_2^+$

CH_3-$C_2H_2^+$	atomic no.	x	y	z
MP2/6-311++G(d,p)	6	-0.496561000	0.696938000	0.000024000
	1	-0.523646000	1.772848000	0.000010000
	6	-0.849223000	-0.491806000	-0.000021000
	1	-1.205995000	-1.506866000	-0.000029000
	6	0.987048000	-0.122231000	-0.000050000
	1	1.429771000	0.228849000	0.929854000
	1	1.429708000	0.228216000	-0.930185000
	1	1.022577000	-1.220453000	0.000632000
B3LYP/ aug-cc-pVTZ	6	0.325875000	0.673075000	-0.000006000
	1	0.310449000	1.749789000	0.000008000
	6	1.035155000	-0.341979000	0.000009000
	1	1.565189000	-1.276948000	-0.000015000
	6	-1.018319000	-0.214196000	0.000000000
	1	-1.524715000	0.063292000	-0.921828000
	1	-1.524816000	0.063435000	0.921730000
	1	-0.882371000	-1.300961000	0.000089000

Table S1d. Coordinates of the optimised geometry of B_3^+

B_3^+	atomic no.	x	y	z
MP2/6-311++G(d,p)	5	0.809859000	0.467574000	0.467574000
	5	-0.809859000	0.467268000	0.467268000
	5	0.000000000	-0.934842000	-0.934842000
B3LYP/ aug-cc-pVTZ	5	0.779388000	-0.449986000	0.000000000
	5	-0.779388000	-0.449952000	0.000000000
	5	0.000000000	0.899938000	0.000000000

Table S1e. Coordinates of the optimised geometry of $C_3H_3^+$

$C_3H_3^+$	atomic no.	x	y	z
MP2/6-311++G(d,p)	6	-0.686124000	0.396575000	-0.000013000
	6	0.686501000	0.395923000	-0.000013000
	6	-0.000377000	-0.792484000	-0.000006000
	1	-1.623730000	0.938430000	-0.000029000
	1	1.624621000	0.936886000	-0.000028000
	1	-0.000892000	-1.875401000	0.000242000
B3LYP/ aug-cc-pVTZ	6	-0.723081000	0.302946000	-0.000015000
	6	0.623895000	0.474738000	-0.000015000
	6	0.099181000	-0.777673000	-0.000013000
	1	-1.719062000	0.720188000	-0.000004000
	1	1.483285000	1.128586000	-0.000003000
	1	0.235809000	-1.848842000	0.000267000

Table S1f. Coordinates of the optimised geometry of H_3^+

H_3^+	atomic no.	x	y	z
MP2/6-311++G(d,p)	1	0.000000000	-0.504607000	0.000000000
	1	-0.437019000	0.252295000	0.000000000
	1	0.437019000	0.252312000	0.000000000
B3LYP/ aug-cc-pVTZ	1	0.440091000	-0.254046000	0.000000000
	1	-0.440091000	-0.254071000	0.000000000
	1	0.000000000	0.508117000	0.000000000

Table S1g. Coordinates of the optimised geometry of 2-norbornyl$^+$

2-norbornyl$^+$	atomic no.	x	y	z
MP2/6-311++G(d,p)	6	-0.159592000	-1.395414000	-0.000301000
	6	-1.125629000	0.001038000	-0.699744000
	6	0.975841000	0.677280000	0.000031000
	6	1.259575000	-0.834173000	-0.000368000
	1	-0.476331000	-1.976742000	0.873001000
	1	-0.476486000	-1.976054000	-0.874018000
	1	1.806803000	-1.152782000	0.889636000
	1	1.806594000	-1.152421000	-0.890628000
	6	0.020721000	0.849442000	-1.195141000
	1	-0.339709000	1.882227000	-1.291409000
	1	0.427640000	0.519021000	-2.153382000
	6	-1.125382000	0.000584000	0.700023000
	1	-1.944306000	-0.376659000	1.305372000
	6	0.021068000	0.848793000	1.195570000
	1	-0.339377000	1.881509000	1.292505000
	1	0.428295000	0.517870000	2.153505000
	1	-1.944727000	-0.375870000	-1.305071000
	1	1.851993000	1.324601000	0.000063000
B3LYP/ aug-cc-pVTZ	6	-0.474700000	1.355535000	-0.002554000
	6	1.042039000	0.456227000	-0.693087000
	6	-0.599978000	-1.020444000	0.000247000
	6	-1.500109000	0.232025000	-0.002960000
	1	-0.433542000	2.006329000	0.868989000
	1	-0.430418000	2.003700000	-0.875894000
	1	-2.135704000	0.278565000	0.878599000
	1	-2.132742000	0.276301000	-0.886778000
	6	0.345765000	-0.779562000	-1.194580000
	1	1.089087000	-1.575375000	-1.300974000
	1	-0.151542000	-0.647522000	-2.152721000

	6	1.039107000	0.458632000	0.695175000
	1	1.615864000	1.142061000	1.301993000
	6	0.340819000	-0.775716000	1.198093000
	1	1.083479000	-1.571285000	1.310371000
	1	-0.160624000	-0.640445000	2.153640000
	1	1.620685000	1.138010000	-1.299984000
	1	-1.122202000	-1.970526000	0.000757000

Table S1h. Coordinates of the optimised geometry of SiH_5^+

SiH_5^+	atomic no.	x	y	z
MP2/6-311++G(d,p)	14	0.173865000	0.003461000	-0.000220000
	1	-1.660427000	-0.429703000	0.003307000
	1	0.335597000	-0.738909000	-1.242081000
	1	0.226063000	1.459705000	-0.034291000
	1	0.341017000	-0.680654000	1.273879000
	1	-1.676364000	0.341102000	0.002265000
B3LYP/ aug-cc-pVTZ	14	0.176314000	0.003534000	-0.000200000
	1	-1.676098000	-0.435333000	0.003219000
	1	0.336761000	-0.740019000	-1.254640000
	1	0.220348000	1.471679000	-0.030808000
	1	0.341860000	-0.687758000	1.283005000
	1	-1.691270000	0.341956000	0.002021000

Table S1i. Coordinates of the optimised geometry of $Al_2H_7^-$

$Al_2H_7^-$	atomic no.	x	y	z
MP2/6-311++G(d,p)	13	1.628085000	-0.000147000	-0.001235000
	1	2.336666000	-0.727411000	-1.250949000
	1	1.682029000	-0.837602000	1.366354000
	1	1.998670000	1.556810000	0.143025000
	13	-1.628107000	0.000134000	-0.001219000
	1	-2.329279000	0.783636000	-1.220662000
	1	-2.014655000	-1.557572000	0.081344000
	1	-1.673102000	0.782786000	1.398673000
	1	-0.000044000	-0.000486000	-0.485894000
B3LYP/ aug-cc-pVTZ	13	-1.697354000	0.000006000	-0.000168000
	1	-2.177254000	0.724866000	-1.358492000
	1	-1.995006000	0.839840000	1.341887000
	1	-2.085003000	-1.561927000	0.088842000
	13	1.697382000	-0.000005000	-0.000181000

	1	2.175900000	-0.838385000	-1.291988000
	1	2.087479000	1.563253000	-0.043957000
	1	1.993523000	-0.723183000	1.408462000
	1	-0.000002000	-0.004481000	-0.140217000