Supporting Information: Assessment of Empirical and Semi-Empirical van der Waals Methods for Halide Perovskites into Density Functional Theory Approach

Celso R. C. Rêgo,*,† Maurício J. Piotrowski,*,‡ Alexandre C. Dias,*,¶ Luís Octavio de Araújo,*,§ Diego Guedes-Sobrinho,*,§ and Wolfgang Wenzel*,†

†Institute of Nanotechnology Hermann-von-Helmholtz-Platz, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany

‡Department of Physics, Federal University of Pelotas, PO Box 354, 96010-900, Pelotas, RS, Brazil ¶Physical Institute, University of Brasília, Brasília, DF, 70919-970, Brazil §Chemistry Department, Federal University of Paraná, CEP 81531-980, Curitiba, Brazil

E-mail: celso.rego@kit.edu; mauriciomjp@gmail.com; alexandre.dias@unb.br; luisaraujo@ufpr.br; guedessobrinho@ufpr.br; wolfgang.wenzel@kit.edu

Table S1: Ionic radii (r_{ion}) for the X (N, P, As, and Sb), I, and Pb chemical elements, considering the respective charge state (CS) and coordination number (CN), from the literature.^{1,2}

Element (Z)	Ion	CS	CN	r _{ion} (pm)
N (7)	N^{-3}	-3	4	146
P (15)	P^{-3}	-3	4	212
As (33)	As^{-3}	-3	4	222
Sb (51)	Sb^{-3}	-3	4	245
I (53)	I^{-1}	-1	6	220
Pb (82)	Pb^{+2}	2	6	119

Table S2: Pauling electronegativity for the chemical elements involved in the XH_4PbI_3 and $CH_3XH_3PbI_3$ (X = N, P, As, and Sb) constitution, from the literature.³

	Н	С	N	P	As	Sb	I	Pb
Atomic number	1	6	7	15	33	51	53	82
Electronegativity	2.20	2.55	3.04	2.19	2.18	2.05	2.66	1.80

Table S3: For XH_4PbI_3 : the tolerance factor, t, is obtained from the X-H average bond lengths, $d_{av,X-H}$, and the ionic radii of XH_4^+ , r_{XH_4} (estimated by $r_{XH_4} = \sqrt{2}d_{av,X-H}$). For $CH_3XH_3PbI_3$: the t factor is obtained by two ways: (i) from the C-X bond lengths, d_{C-X} , and the ionic radii of $CH_3XH_3^+$, $r_{CH_3XH_3}$ (estimated by $r_{CH_3XH_3} = 0.5d_{C-X} + r_{X,ion}$); and (ii) from the distance between the center of mass (CM) of the molecule and the atom with the largest distance to CM, except the H atoms, d_{CM} , and the ionic radii of $CH_3XH_3^+$, $r_{CH_3XH_3}$ (estimated by $r_{CH_3XH_3} = d_{CM} + r_{X,ion}$). For both sets, X = N, P, As, and Sb, and all structures are optimized within empirical (D2, D3, and D3BJ), semi-empirical (TS, TSSCS, MBD, and dDsC), and without (std.) vdW corrections.

System		std.	D2	D3	D3BJ	TS	TSSCS	MBD	dDsC
	d _{av,N-H} (pm)	104.25	104.27	104.13	104.29	104.52	103.81	103.87	103.80
NH ₄ PbI ₃	$r_{\rm NH_4}$ (pm)	147.44	147.46	147.27	147.49	147.81	146.81	146.90	146.79
4 3	t	0.7664	0.7665	0.7661	0.7665	0.7672	0.7651	0.7653	0.7651
	$d_{av,P-H}$ (pm)	142.31	141.94	142.27	142.36	141.96	142.09	142.31	142.12
PH_4PbI_3	r_{PH_4} (pm)	201.26	200.73	201.20	201.33	200.76	200.95	201.26	200.99
7 3	t	0.8787	0.8776	0.8786	0.8788	0.8776	0.8780	0.8787	0.8781
	$d_{av, As-H}$ (pm)	152.20	151.51	151.88	152.19	151.77	152.02	152.20	151.84
AsH_4PbI_3	r_{AsH_4} (pm)	215.24	214.26	214.78	215.22	214.64	214.99	215.24	214.73
	t	0.9078	0.9058	0.9069	0.9078	0.9066	0.9073	0.9078	0.9068
	$d_{av, Sb-H}$ (pm)	170.41	169.85	170.37	170.48	169.96	170.09	169.70	169.31
SbH ₄ PbI ₃	r_{SbH_4} (pm)	241.00	240.21	240.93	241.10	240.36	240.54	240.00	239.44
	t	0.9616	0.9599	0.9614	0.9618	0.9602	0.9606	0.9595	0.9583
System (by (i))		std.	D2	D3	D3BJ	TS	TSSCS	MBD	dDsC
	$d_{\text{C-N}} \text{ (pm)}$	149.11	149.32	148.97	148.96	149.10	149.02	148.97	148.87
CH ₃ NH ₃ PbI ₃	$r_{\text{CH}_3\text{NH}_3}$ (pm)	220.56	220.66	220.49	220.48	220.55	220.51	220.49	220.43
	t	0.9189	0.9192	0.9188	0.9188	0.9189	0.9188	0.9188	0.9187
	$d_{\mathrm{C-P}}$ (pm)	179.49	179.45	179.43	179.50	179.21	179.21	179.42	179.23
$CH_3PH_3PbI_3$	$r_{\text{CH}_3\text{PH}_3}$ (pm)	301.74	301.72	301.72	301.75	301.61	301.60	301.71	301.61
	t	1.0883	1.0882	1.0882	1.0883	1.0880	1.0880	1.0882	1.0880
	$d_{\mathrm{C-As}}$ (pm)	192.80	192.82	192.64	192.54	192.62	192.56	192.77	192.45
$CH_3AsH_3PbI_3$	$r_{\text{CH}_3\text{AsH}_3}$ (pm)	318.40	318.41	318.32	318.27	318.31	318.28	318.38	318.22
	t	1.1230	1.1230	1.1228	1.1228	1.1228	1.1228	1.1230	1.1227
	$d_{\text{C-Sb}}$ (pm)	212.23	212.42	211.72	211.78	211.46	211.84	211.84	211.71
$CH_3SbH_3PbI_3$	$r_{\text{CH}_3\text{SbH}_3}$ (pm)	351.11	351.21	350.86	350.89	350.73	350.92	350.92	350.86
	t	1.2659	1.2662	1.2654	1.2655	1.2651	1.2655	1.2655	1.2654
System (by (ii))		std.	D2	D3	D3BJ	TS	TSSCS	MBD	dDsC
	d_{CM} (pm)	78.64	79.44	79.25	79.24	78.64	78.62	78.58	78.53
$CH_3NH_3PbI_3$	$r_{\text{CH}_3\text{NH}_3}$ (pm)	224.64	225.44	225.25	225.24	224.64	224.62	224.58	224.53
	t	0.9275	0.9291	0.9287	0.9287	0.9275	0.9274	0.9273	0.9272
	d_{CM} (pm)	111.97	111.98	111.96	111.98	111.84	111.83	111.94	111.84
$CH_3PH_3PbI_3$	$r_{\text{CH}_3\text{PH}_3}$ (pm)	323.97	323.98	323.96	323.98	323.84	323.83	323.94	323.84
	t	1.1346	1.1347	1.1346	1.1347	1.1344	1.1344	1.1346	1.1344
	d_{CM} (pm)	102.77	102.81	102.71	102.62	102.47	102.44	102.55	102.38
$CH_3AsH_3PbI_3$	$r_{\text{CH}_3\text{AsH}_3}$ (pm)	324.77	324.81	324.71	324.62	324.47	324.44	324.55	324.38
	t	1.1363	1.1364	1.1362	1.1360	1.1357	1.1356	1.1358	1.1355
	d_{CM} (pm)	70.40	70.50	70.13	70.16	69.99	70.20	70.20	70.22
$CH_3SbH_3PbI_3$	$r_{\text{CH}_3\text{AsH}_3}$ (pm)	315.40	315.50	315.13	315.16	314.99	315.20	315.20	315.22
	t	1.1168	1.1170	1.1162	1.1163	1.1159	1.1163	1.1163	1.1164

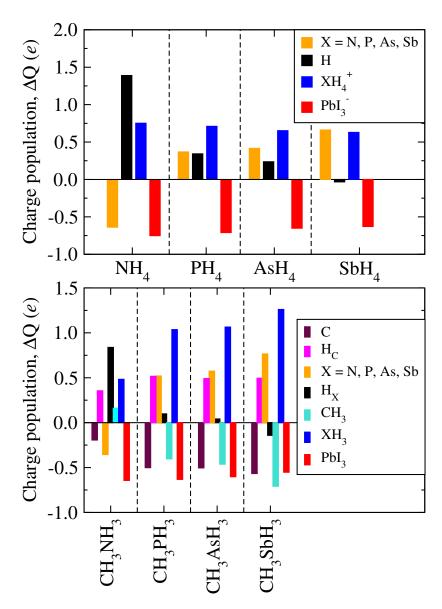


Figure S1: Partial charges computed for X (N, P, As, Sb), C, H_C , H_X , XH_4 , CH_3 , XH_3 , and PbI_3 via density-derived electrostatic and chemical (DDEC6) method for the XH_4PbI_3 and $CH_3XH_3PbI_3$ MHPs.

Table S4: Equatorial (equat.) and apical (api.) Pb–I bonds and Pb–I–Pb angles as local structure parameters for XH_4PbI_3 (X=N,P,As, and Sb) perovskites obtained within empirical (D2, D3, and D3BJ), semi-empirical (TS, TSSCS, MBD, and dDsC), and without (std.) vdW corrections. The α , β , and γ angles of the unit cell are indicated for every calculation mode.

Facility	Sys.	vdW	Pb-I be	angle (deg)	Uni	t cell	(deg)		
D2 3.13-3.15 3.14-3.15 158-180 158-158 90 90 90 90 90 3.13-3.15 3.15-3.15 158-180 158-158 90 90 90 90 91 158-158 158-158 90 90 90 91 158-158 158-158 90 90 91 158-158 179-179 179-1			equat.	api.	equat.	api.	α	β	γ
Hart Day Da		std.	3.18–3.20	3.19–3.19	155–179	155–155	90	90	90
TS Silo S		D2	3.13-3.15	3.14-3.15	158-180	158-158	90	90	90
HSCS 3.12-3.23 3.15-3.15 169-179 179-179 90 90 89 MBD 3.10-3.21 3.13-3.13 167-179 178-178 90 90 89 MBD 3.11-3.20 3.12-3.12 167-179 178-178 90 90 89 REA equat. api. equat. api. α β γ std. 3.16-3.19 3.19-3.19 175-180 175-175 90 90 90 D2 3.09-3.11 3.11-3.11 180-180 180-180 90 90 90 D3 3.11-3.13 3.13-3.13 178-180 177-177 90 90 90 D3 3.10-3.12 3.12-3.12 176-180 176-176 90 90 90 TS 3.10-3.16 3.14-3.14 179-180 179-179 90 90 90 MBD 3.12-3.15 3.15-3.16 173-180 173-173 90 90 90 SDSC 3.12-3.15 3.15-3.15 175-179 174-174 90 90 90 MBD 3.10-3.12 3.20-3.22 172-178 169-169 90 90 90 D3 3.10-3.15 3.14-3.15 178-180 177-177 90 90 90 D3 3.10-3.15 3.14-3.15 178-180 177-177 90 90 90 D3 3.10-3.15 3.14-3.15 178-180 177-177 90 90 90 D3 3.10-3.15 3.15-3.15 178-180 177-177 90 90 90 D3 3.10-3.14 3.13-3.14 176-180 173-173 90 90 90 MBD 3.12-3.16 3.16-3.16 173-178 175-175 90 90 90 MBD 3.12-3.16 3.16-3.16 173-178 175-175 90 90 90 D3 3.12-3.16 3.16-3.16 175-180 175-175 90 90 90 MBD 3.12-3.16 3.16-3.16 175-180 175-175 90 90 90 D3 3.12-3.16 3.16-3.16 175-180 175-175 90 90 90 MBD 3.12-3.16 3.16-3.16 175-180 175-175 90 90 90 MBD 3.11-3.16 3.16-3.16 175-180 175-175 90 90 90 90 MBD 3.11-3.16 3.16-3.16 175-180 175-175 90 90 90 90 90 90 90 9	, φ	D3	3.13-3.15	3.15-3.15	158-180	158-158	90	90	90
HSCS 3.12-3.23 3.15-3.15 169-179 179-179 90 90 89 MBD 3.10-3.21 3.13-3.13 167-179 178-178 90 90 89 MBD 3.11-3.20 3.12-3.12 167-179 178-178 90 90 89 REA equat. api. equat. api. α β γ std. 3.16-3.19 3.19-3.19 175-180 175-175 90 90 90 D2 3.09-3.11 3.11-3.11 180-180 180-180 90 90 90 D3 3.11-3.13 3.13-3.13 178-180 177-177 90 90 90 D3 3.10-3.12 3.12-3.12 176-180 176-176 90 90 90 TS 3.10-3.16 3.14-3.14 179-180 179-179 90 90 90 MBD 3.12-3.15 3.15-3.16 173-180 173-173 90 90 90 SDSC 3.12-3.15 3.15-3.15 175-179 174-174 90 90 90 MBD 3.10-3.12 3.20-3.22 172-178 169-169 90 90 90 D3 3.10-3.15 3.14-3.15 178-180 177-177 90 90 90 D3 3.10-3.15 3.14-3.15 178-180 177-177 90 90 90 D3 3.10-3.15 3.14-3.15 178-180 177-177 90 90 90 D3 3.10-3.15 3.15-3.15 178-180 177-177 90 90 90 D3 3.10-3.14 3.13-3.14 176-180 173-173 90 90 90 MBD 3.12-3.16 3.16-3.16 173-178 175-175 90 90 90 MBD 3.12-3.16 3.16-3.16 173-178 175-175 90 90 90 D3 3.12-3.16 3.16-3.16 175-180 175-175 90 90 90 MBD 3.12-3.16 3.16-3.16 175-180 175-175 90 90 90 D3 3.12-3.16 3.16-3.16 175-180 175-175 90 90 90 MBD 3.12-3.16 3.16-3.16 175-180 175-175 90 90 90 MBD 3.11-3.16 3.16-3.16 175-180 175-175 90 90 90 90 MBD 3.11-3.16 3.16-3.16 175-180 175-175 90 90 90 90 90 90 90 9	PbI	D3BJ	3.14–3.15	3.14–3.16	154–178	154–154	90	90	91
HSCS 3.12-3.23 3.15-3.15 169-179 179-179 90 90 89 MBD 3.10-3.21 3.13-3.13 167-179 178-178 90 90 89 MBD 3.11-3.20 3.12-3.12 167-179 178-178 90 90 89 REA equat. api. equat. api. α β γ std. 3.16-3.19 3.19-3.19 175-180 175-175 90 90 90 D2 3.09-3.11 3.11-3.11 180-180 180-180 90 90 90 D3 3.11-3.13 3.13-3.13 178-180 177-177 90 90 90 D3 3.10-3.12 3.12-3.12 176-180 176-176 90 90 90 TS 3.10-3.16 3.14-3.14 179-180 179-179 90 90 90 MBD 3.12-3.15 3.15-3.16 173-180 173-173 90 90 90 SDSC 3.12-3.15 3.15-3.15 175-179 174-174 90 90 90 MBD 3.10-3.12 3.20-3.22 172-178 169-169 90 90 90 D3 3.10-3.15 3.14-3.15 178-180 177-177 90 90 90 D3 3.10-3.15 3.14-3.15 178-180 177-177 90 90 90 D3 3.10-3.15 3.14-3.15 178-180 177-177 90 90 90 D3 3.10-3.15 3.15-3.15 178-180 177-177 90 90 90 D3 3.10-3.14 3.13-3.14 176-180 173-173 90 90 90 MBD 3.12-3.16 3.16-3.16 173-178 175-175 90 90 90 MBD 3.12-3.16 3.16-3.16 173-178 175-175 90 90 90 D3 3.12-3.16 3.16-3.16 175-180 175-175 90 90 90 MBD 3.12-3.16 3.16-3.16 175-180 175-175 90 90 90 D3 3.12-3.16 3.16-3.16 175-180 175-175 90 90 90 MBD 3.12-3.16 3.16-3.16 175-180 175-175 90 90 90 MBD 3.11-3.16 3.16-3.16 175-180 175-175 90 90 90 90 MBD 3.11-3.16 3.16-3.16 175-180 175-175 90 90 90 90 90 90 90 9	, HN								
Hart									
Std. 3.16-3.12 3.15-3.15 175-179 174-174 90 90 90 90 90 90 90 9									
Std. 3.16-3.19 3.19-3.19 175-180 175-175 90 90 90 90 90 90 90 9		dDsC	3.11–3.20	3.12–3.12	167–179	178–178	90	90	89
D2 3.09-3.11 3.11-3.11 180-180 180-180 90 90 90 90 90 90 90			equat.	api.	equat.	api.	α	β	γ
D3 3.11-3.13 3.13-3.13 178-180 177-177 90 90 90 90		std.	3.16-3.19	3.19-3.19	175–180	175–175	90	90	90
D3BJ 3.10-3.12 3.12-3.12 176-180 176-176 90 90 90 90 TSSCS 3.14-3.18 3.18-3.18 176-179 176-176 90 90 90 90 MBD 3.12-3.15 3.15-3.16 173-180 173-173 90 90 90 90 SDSC 3.12-3.15 3.15-3.15 175-179 174-174 90 90 90 90 90 90 90 9		D2	3.09-3.11		180–180	180–180	90	90	90
TSSCS 3.14-3.18 3.18-3.18 176-179 176-176 90 90 90 90 8DsC 3.12-3.15 3.15-3.16 173-180 173-173 90 90 90 90 90 90 90 9	3_					177–177			
TSSCS 3.14-3.18 3.18-3.18 176-179 176-176 90 90 90 90 8DsC 3.12-3.15 3.15-3.16 173-180 173-173 90 90 90 90 90 90 90 9	$^{ ext{PbJ}}$	D3BJ	3.10–3.12	3.12–3.12	176–180	176–176	90	90	90
TSSCS 3.14-3.18 3.18-3.18 176-179 176-176 90 90 90 90 8DsC 3.12-3.15 3.15-3.16 173-180 173-173 90 90 90 90 90 90 90 9	7 Hd		3.10-3.16		179–180	179–179	90	90	90
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$, ,	TSSCS	3.14–3.18	3.18-3.18	176–179	176–176	90	90	90
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		MBD		3.15–3.16	173–180	173–173	90	90	90
std. 3.16–3.21 3.20–3.22 172–178 169–169 90 90 90 D2 3.09–3.12 3.10–3.12 178–179 180–180 90 90 90 D3 3.10–3.15 3.14–3.15 178–180 177–177 90 90 90 D3BJ 3.10–3.14 3.13–3.14 176–180 173–173 90 90 90 TS 3.12–3.15 3.15–3.15 178–180 178–178 90 90 90 MBD 3.12–3.16 3.16–3.16 173–178 175–175 90 90 90 MBD 3.12–3.16 3.16–3.16 173–178 175–175 90 90 90 Std. 3.17–3.21 3.21–3.21 179–180 179–179 90 90 90 D2 3.09–3.13 3.12–3.12 169–180 169–169 90 90 90 D3 3.12–3.16 3.16–3.16 175–180 175–175 90 90 90		sDsC	3.12–3.15	3.15–3.15	175–179	174–174	90	90	90
D2 3.09-3.12 3.10-3.12 178-179 180-180 90 90 90 90 D3 3.10-3.15 3.14-3.15 178-180 177-177 90 90 90 90 D3BJ 3.10-3.14 3.13-3.14 176-180 173-173 90 90 90 MBD 3.12-3.15 3.15-3.15 178-180 178-178 90 90 90 MBD 3.12-3.16 3.16-3.16 173-178 175-175 90 90 90 90 MBD 3.12-3.17 3.17-3.17 172-180 173-173 90 90 89 90 90 90 90 90			equat.	api.	equat.	api.	α	β	γ
EAT D3 3.10-3.15 3.14-3.15 178-180 177-177 90 90 90 HZ D3BJ 3.10-3.14 3.13-3.14 176-180 173-173 90 90 90 TS 3.12-3.15 3.15-3.15 178-180 178-178 90 90 90 MBD 3.12-3.16 3.16-3.19 174-178 175-175 90 90 90 MBD 3.12-3.16 3.16-3.16 173-178 175-175 90 90 90 89 equat. api. equat. api. α β γ Std. 3.17-3.21 3.21-3.21 179-180 179-179 90 90 90 D2 3.09-3.13 3.12-3.12 169-180 169-169 90 90 90 D3 3.12-3.16 3.16-3.16 175-180 175-175 90 90 90 B0 D3BJ 3.11-3.16 3.16-3.16 175-180 175-175 90 90 90		std.	3.16-3.21	3.20-3.22	172-178	169-169	90	90	90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		D2	3.09-3.12	3.10-3.12	178–179	180-180	90	90	90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	I_3	D3	3.10-3.15	3.14-3.15	178-180	177–177	90	90	90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Pb	D3BJ	3.10–3.14	3.13–3.14	176–180	173–173	90	90	90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	√sH	TS	3.12-3.15	3.15-3.15	178-180	178-178	90	90	90
$\frac{\text{dDsC}}{\text{Equat.}} \begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	TSSCS			174–178		90	90	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		MBD			173–178	175–175			
std. 3.17–3.21 3.21–3.21 179–180 179–179 90 90 90 90 D2 3.09–3.13 3.12–3.12 169–180 169–169 90 90 90 90 D3 3.12–3.16 3.16–3.16 175–180 175–175 90 90 90 P0 D3BJ 3.10–3.14 3.14–3.14 174–180 174–174 90 90 89 TSSCS 3.14–3.19 3.19–3.19 176–180 178–178 90 90 90 MBD 3.11–3.16 3.16–3.16 172–179 172–172 90 90 90		dDsC	3.12–3.17	3.17–3.17	172–180	173–173	90	90	89
D2 3.09-3.13 3.12-3.12 169-180 169-169 90 90 90 90 D3 3.12-3.16 3.16-3.16 175-180 175-175 90 90 90 D3BJ 3.10-3.14 3.14-3.14 174-180 174-174 90 90 89 TSSCS 3.14-3.19 3.19-3.19 176-180 178-178 90 90 90 MBD 3.11-3.16 3.16-3.16 172-179 172-172 90 90 90			equat.	api.	equat.	api.	α	β	γ
TSSCS 3.14-3.16 3.16-3.16 175-180 175-175 90 90 90 90 MBD 3.11-3.16 3.16-3.16 175-180 175-175 90 90 90 90 MBD 3.11-3.16 3.16-3.16 175-180 175-175 90 90 90 90 90 MBD 3.11-3.16 3.16-3.16 172-179 172-172 90 90 90		std.	3.17-3.21		179–180	179–179	90	90	90
MBD 3.11–3.16 3.16–3.16 172–179 172–172 90 90 90							90	90	90
MBD 3.11–3.16 3.16–3.16 172–179 172–172 90 90 90	\mathbf{I}_3		3.12-3.16	3.16-3.16	175–180	175–175		90	
MBD 3.11–3.16 3.16–3.16 172–179 172–172 90 90 90	Pb	D3BJ	3.10–3.14	3.14–3.14	174–180	174–174	90	90	89
MBD 3.11–3.16 3.16–3.16 172–179 172–172 90 90 90	Hq:	TS	3.11-3.16	3.16-3.16	175–180	175–175	90	90	90
	6 2	TSSCS	3.14-3.19	3.19-3.19	176–180	178–178	90	90	90
dDsC 3.12–3.16 3.16–3.16 170–180 170–170 90 90 90		MBD	3.11-3.16	3.16-3.16	172–179	172–172	90	90	90
		dDsC	3.12–3.16	3.16–3.16	170–180	170–170	90	90	90

Table S5: Equatorial (equat.) and apical (api.) Pb–I bonds and Pb–I–Pb angles as local structure parameters for $CH_3XH_3PbI_3$ (X = N, P, As, and Sb) perovskites obtained within empirical (D2, D3, and D3BJ), semi-empirical (TS, TSSCS, MBD, and dDsC), and without (std.) vdW corrections. The α , β , and γ angles of the unit cell are indicated for every calculation mode.

std. api. equat. api. equat. api. α β γ std. 3.07-3.35 3.20-3.27 168-172 169-169 90 89 90 D2 3.06-3.25 3.13-3.13 160-164 160-160 90 89 90 D3 3.08-3.22 3.16-3.19 168-172 172-172 90 89 90 D3BJ 3.07-3.20 3.15-3.18 168-172 172-172 90 90 90 TSSCS 3.04-3.37 3.20-3.24 171-176 169-169 90 89 90 MBD 3.06-3.30 3.18-3.21 170-174 169-169 90 89 90 MBD 3.06-3.30 3.19-3.23 166-171 170-170 90 89 90 std. 3.21-3.22 3.23-3.23 179-179 180-180 90 87 90 Bar D2 3.15-3.16 3.13-3.13 178-180 179-179 90 87 90 <t< th=""><th>Sys.</th><th>vdW</th><th>Pb-I b</th><th>ond (Å)</th><th>Pb-I-Pb a</th><th>angle (deg)</th><th>Uni</th><th>t cell</th><th>(deg)</th></t<>	Sys.	vdW	Pb-I b	ond (Å)	Pb-I-Pb a	angle (deg)	Uni	t cell	(deg)
D2 3.06-3.25 3.13-3.13 160-164 160-160 90 89 90			equat.	api.	equat.	api.	α	β	γ
D2 3.06-3.25 3.13-3.13 160-164 160-160 90 89 90		std.	3.07-3.35	3.20-3.27	168–172	169–169	90	89	90
TSSCS 3.04-3.37 3.20-3.24 171-176 169-169 90 89 90 MBD 3.06-3.30 3.19-3.23 166-171 170-170 90 89 90 MBD 3.10-3.23 3.18-3.21 168-172 171-171 90 89 90 Std. 3.21-3.22 3.23-3.23 179-179 180-180 90 87 90 MBD 3.15-3.16 3.13-3.13 178-180 179-179 90 87 90 MBD 3.16-3.18 3.15-3.16 179-179 180-180 90 87 90 MBD 3.18-3.20 3.19-3.19 180-180 180-180 90 88 90 MBD 3.18-3.20 3.19-3.11 180-180 180-180 90 86 90 MBD 3.18-3.20 3.17-3.17 180-180 180-180 90 86 90 MBD 3.13-3.18 3.14-3.14 178-178 180-180 90 86 90 MBD 3.13-3.19 3.15-3.17 177-177 177-177 90 86 90 MBD 3.19-3.21 3.20-3.20 177-178 179-179 90 85 90 MBD 3.19-3.21 3.20-3.20 177-178 180-180 90 85 90 MBD 3.19-3.21 3.20-3.20 177-178 180-180 90 85 90 MBD 3.19-3.21 3.19-3.19 180-180 180-180 90 85 90 MBD 3.19-3.21 3.19-3.19 180-180 180-180 90 85 90 MBD 3.19-3.21 3.10-3.23 171-175 165-165 90 83 90 MBD 3.18-3.23 3.13-3.19 174-179 173-173 90 84 90 MBD 3.19-3.26 3.14-3.23 174-180 173-173 90 84 90 MBD 3.19-3.26 3.17-3.23 170-177 174-174 90 85 90 MBD 3.19-3.26 3.17-3.23	bI_3	D2		3.13-3.13			90		
TSSCS 3.04-3.37 3.20-3.24 171-176 169-169 90 89 90 MBD 3.06-3.30 3.19-3.23 166-171 170-170 90 89 90 MBD 3.10-3.23 3.18-3.21 168-172 171-171 90 89 90 Std. 3.21-3.22 3.23-3.23 179-179 180-180 90 87 90 MBD 3.15-3.16 3.13-3.13 178-180 179-179 90 87 90 MBD 3.16-3.18 3.15-3.16 179-179 180-180 90 87 90 MBD 3.18-3.20 3.19-3.19 180-180 180-180 90 88 90 MBD 3.18-3.20 3.19-3.11 180-180 180-180 90 86 90 MBD 3.18-3.20 3.17-3.17 180-180 180-180 90 86 90 MBD 3.13-3.18 3.14-3.14 178-178 180-180 90 86 90 MBD 3.13-3.19 3.15-3.17 177-177 177-177 90 86 90 MBD 3.19-3.21 3.20-3.20 177-178 179-179 90 85 90 MBD 3.19-3.21 3.20-3.20 177-178 180-180 90 85 90 MBD 3.19-3.21 3.20-3.20 177-178 180-180 90 85 90 MBD 3.19-3.21 3.19-3.19 180-180 180-180 90 85 90 MBD 3.19-3.21 3.19-3.19 180-180 180-180 90 85 90 MBD 3.19-3.21 3.10-3.23 171-175 165-165 90 83 90 MBD 3.18-3.23 3.13-3.19 174-179 173-173 90 84 90 MBD 3.19-3.26 3.14-3.23 174-180 173-173 90 84 90 MBD 3.19-3.26 3.17-3.23 170-177 174-174 90 85 90 MBD 3.19-3.26 3.17-3.23	[3P]	D3	3.08-3.22	3.16-3.19	168-172	172-172	90	89	90
TSSCS 3.04-3.37 3.20-3.24 171-176 169-169 90 89 90 MBD 3.06-3.30 3.19-3.23 166-171 170-170 90 89 90 MBD 3.10-3.23 3.18-3.21 168-172 171-171 90 89 90 Std. 3.21-3.22 3.23-3.23 179-179 180-180 90 87 90 MBD 3.15-3.16 3.13-3.13 178-180 179-179 90 87 90 MBD 3.16-3.18 3.15-3.16 179-179 180-180 90 87 90 MBD 3.18-3.20 3.19-3.19 180-180 180-180 90 88 90 MBD 3.18-3.20 3.19-3.11 180-180 180-180 90 86 90 MBD 3.18-3.20 3.17-3.17 180-180 180-180 90 86 90 MBD 3.13-3.18 3.14-3.14 178-178 180-180 90 86 90 MBD 3.13-3.19 3.15-3.17 177-177 177-177 90 86 90 MBD 3.19-3.21 3.20-3.20 177-178 179-179 90 85 90 MBD 3.19-3.21 3.20-3.20 177-178 180-180 90 85 90 MBD 3.19-3.21 3.20-3.20 177-178 180-180 90 85 90 MBD 3.19-3.21 3.19-3.19 180-180 180-180 90 85 90 MBD 3.19-3.21 3.19-3.19 180-180 180-180 90 85 90 MBD 3.19-3.21 3.10-3.23 171-175 165-165 90 83 90 MBD 3.18-3.23 3.13-3.19 174-179 173-173 90 84 90 MBD 3.19-3.26 3.14-3.23 174-180 173-173 90 84 90 MBD 3.19-3.26 3.17-3.23 170-177 174-174 90 85 90 MBD 3.19-3.26 3.17-3.23	HZ.	D3BJ	3.07-3.20	3.15-3.18	168–172	172-172	90	90	90
MBD 3.06-3.30 3.19-3.23 166-171 170-170 90 89 90	CH	TS	3.06-3.30	3.18-3.21	170–174	169–169	90	88	90
Hart Hart		TSSCS	3.04-3.37	3.20-3.24	171–176	169–169	90	89	90
std. 3.21-3.22 3.23-3.23 179-179 180-180 90 87 90 Hearth D2 3.15-3.16 3.13-3.13 178-180 179-179 90 87 90 Hearth D3 3.16-3.18 3.15-3.16 179-179 180-180 90 87 90 B3BJ 3.15-3.16 3.15-3.16 179-179 180-180 90 87 90 TS 3.18-3.20 3.19-3.19 180-180 180-180 90 86 90 MBD 3.18-3.20 3.18-3.18 180-180 180-180 90 86 90 MBD 3.18-3.20 3.17-3.17 180-180 180-180 90 86 90 MBD 3.18-3.20 3.17-3.17 180-180 180-180 90 86 90 MBC 3.18-3.20 3.17-3.17 180-180 180-180 90 86 90 Heart api. equat. api. api. api. y <td></td> <td>MBD</td> <td>3.06-3.30</td> <td>3.19-3.23</td> <td>166–171</td> <td>170-170</td> <td>90</td> <td>89</td> <td>90</td>		MBD	3.06-3.30	3.19-3.23	166–171	170-170	90	89	90
Std. 3.21-3.22 3.23-3.23 179-179 180-180 90 87 90 90 90 90 90 90 90 9		dDsC	3.10-3.23	3.18-3.21	168–172	171–171	90	89	90
D2 3.15-3.16 3.13-3.13 178-180 179-179 90 87 90 90 90 90 90 90 90 9			equat.	api.	equat.	api.	α	β	γ
TSSCS 3.20-3.22 3.21-3.21 180-180 180-180 90 86 90 MBD 3.18-3.20 3.18-3.17 180-180 180-180 90 86 90 dDsC 3.18-3.20 3.17-3.17 180-180 180-180 90 86 90 80 80 90 90 80 90 90 80 90 90 90 90 90 90 90 90 90 90 90 90 90		std.	3.21-3.22	3.23-3.23	179–179	180-180	90	87	90
TSSCS 3.20-3.22 3.21-3.21 180-180 180-180 90 86 90 MBD 3.18-3.20 3.18-3.17 180-180 180-180 90 86 90 dDsC 3.18-3.20 3.17-3.17 180-180 180-180 90 86 90 80 80 90 90 80 90 90 80 90 90 90 90 90 90 90 90 90 90 90 90 90	bl_3	D2	3.15-3.16	3.13-3.13	178-180	179–179	90	87	90
TSSCS 3.20-3.22 3.21-3.21 180-180 180-180 90 86 90 MBD 3.18-3.20 3.18-3.17 180-180 180-180 90 86 90 dDsC 3.18-3.20 3.17-3.17 180-180 180-180 90 86 90 80 80 90 90 80 90 90 80 90 90 90 90 90 90 90 90 90 90 90 90 90	$_{13}^{ m P}$	D3	3.16-3.18	3.15-3.17	179–179	180-180	90	87	90
TSSCS 3.20-3.22 3.21-3.21 180-180 180-180 90 86 90 MBD 3.18-3.20 3.18-3.17 180-180 180-180 90 86 90 dDsC 3.18-3.20 3.17-3.17 180-180 180-180 90 86 90 80 80 90 90 80 90 90 80 90 90 90 90 90 90 90 90 90 90 90 90 90	3 PE	D3BJ	3.15–3.16	3.15–3.16	179–179	180–180	90	88	90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	CH	TS	3.18-3.20	3.19-3.19	180-180	180-180	90	86	90
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		TSSCS	3.20-3.22	3.21-3.21	180-180	180-180	90	86	90
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		MBD	3.18-3.20	3.18-3.18	180-180	180-180	90	86	90
Std. 3.19-3.26 3.24-3.25 177-177 177-177 90 86 90 Here D2 3.13-3.18 3.14-3.14 178-178 180-180 90 84 90 D3 3.14-3.22 3.16-3.20 177-178 179-179 90 85 90 D3BJ 3.13-3.19 3.15-3.17 177-178 180-180 90 85 90 TSSCS 3.21-3.23 3.20-3.20 177-178 180-180 90 85 90 MBD 3.19-3.21 3.20-3.20 180-180 180-180 90 85 90 MBC 3.19-3.21 3.19-3.19 180-180 180-180 90 85 90 MBC 3.19-3.21 3.19-3.19 180-180 180-180 90 85 90 MBD 3.16-3.21 3.10-3.23 176-178 177-177 90 86 90 MBD 3.20-3.26 3.14-3.23 174-180 173-173 90 84 90 </td <td></td> <td>dDsC</td> <td>3.18-3.20</td> <td>3.17-3.17</td> <td>180-180</td> <td>180-180</td> <td>90</td> <td>86</td> <td>90</td>		dDsC	3.18-3.20	3.17-3.17	180-180	180-180	90	86	90
Here D2 3.13-3.18 3.14-3.14 178-178 180-180 90 84 90 D3 3.14-3.22 3.16-3.20 177-178 179-179 90 85 90 D3BJ 3.13-3.19 3.15-3.17 177-178 180-180 90 85 90 TSSCS 3.21-3.23 3.23-3.23 180-180 180-180 90 85 90 MBD 3.19-3.21 3.20-3.20 180-180 180-180 90 85 90 dDsC 3.19-3.21 3.19-3.19 180-180 180-180 90 85 90 S5 90 D2 3.16-3.21 3.19-3.19 180-180 180-180 90 85 90 D3 3.20-3.26 3.14-3.23 171-175 165-165 90 83 90 D3BJ 3.18-3.23 3.13-3.19 174-179 173-173 90 84 90 TSSCS 3.19-3.26 3.17-3.23 170-177 174-174 90 85 90 MBD 3.19-3.26 3.17-3.23 170-177 174-174 90 85 90 MBD 3.19-3.26 3.17-3.23 170-177 174-174 90 85 90 MBD 3.19-3.26 3.17-3.23 170-177 174-174 90 85 90			equat.	api.	equat.	api.	α	β	γ
TSSCS 3.21–3.23 3.23–3.23 180–180 180–180 90 86 90 MBD 3.19–3.21 3.20–3.20 180–180 180–180 90 85 90 dDsC 3.19–3.21 3.19–3.19 180–180 180–180 90 85 90 std. 3.26–3.30 3.25–3.25 176–178 177–177 90 86 90 D2 3.16–3.21 3.10–3.23 171–175 165–165 90 83 90 D3BJ 3.18–3.23 3.13–3.19 174–179 173–173 90 84 90 TSSCS 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90 MBD 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90 MBD 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90		std.	3.19-3.26	3.24-3.25	177–177	177–177	90	86	90
TSSCS 3.21–3.23 3.23–3.23 180–180 180–180 90 86 90 MBD 3.19–3.21 3.20–3.20 180–180 180–180 90 85 90 dDsC 3.19–3.21 3.19–3.19 180–180 180–180 90 85 90 std. 3.26–3.30 3.25–3.25 176–178 177–177 90 86 90 D2 3.16–3.21 3.10–3.23 171–175 165–165 90 83 90 D3BJ 3.18–3.23 3.13–3.19 174–179 173–173 90 84 90 TSSCS 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90 MBD 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90 MBD 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90	[19]	D2	3.13-3.18	3.14-3.14	178-178	180-180	90	84	90
TSSCS 3.21–3.23 3.23–3.23 180–180 180–180 90 86 90 MBD 3.19–3.21 3.20–3.20 180–180 180–180 90 85 90 dDsC 3.19–3.21 3.19–3.19 180–180 180–180 90 85 90 std. 3.26–3.30 3.25–3.25 176–178 177–177 90 86 90 D2 3.16–3.21 3.10–3.23 171–175 165–165 90 83 90 D3BJ 3.18–3.23 3.13–3.19 174–179 173–173 90 84 90 TSSCS 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90 MBD 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90 MBD 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90	$_{ m I_3F}$	D3	3.14-3.22	3.16-3.20	177-178	179-179	90	85	90
TSSCS 3.21–3.23 3.23–3.23 180–180 180–180 90 86 90 MBD 3.19–3.21 3.20–3.20 180–180 180–180 90 85 90 dDsC 3.19–3.21 3.19–3.19 180–180 180–180 90 85 90 std. 3.26–3.30 3.25–3.25 176–178 177–177 90 86 90 D2 3.16–3.21 3.10–3.23 171–175 165–165 90 83 90 D3BJ 3.18–3.23 3.13–3.19 174–179 173–173 90 84 90 TSSCS 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90 MBD 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90 MBD 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90	AsF	D3BJ	3.13-3.19	3.15-3.17	177–178	180-180	90	85	90
TSSCS 3.21–3.23 3.23–3.23 180–180 180–180 90 86 90 MBD 3.19–3.21 3.20–3.20 180–180 180–180 90 85 90 dDsC 3.19–3.21 3.19–3.19 180–180 180–180 90 85 90 std. 3.26–3.30 3.25–3.25 176–178 177–177 90 86 90 D2 3.16–3.21 3.10–3.23 171–175 165–165 90 83 90 D3BJ 3.18–3.23 3.13–3.19 174–179 173–173 90 84 90 TSSCS 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90 MBD 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90 MBD 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90	$^{ m CH}_3$	TS	3.20-3.22	3.20-3.20	177–178	180–180	90	85	90
dDsC 3.19–3.21 3.19–3.19 180–180 180–180 90 85 90 equat. api. equat. api. α β γ std. 3.26–3.30 3.25–3.25 176–178 177–177 90 86 90 D2 3.16–3.21 3.10–3.23 171–175 165–165 90 83 90 D3 3.20–3.26 3.14–3.23 174–180 173–173 90 84 90 D3BJ 3.18–3.23 3.13–3.19 174–179 173–173 90 84 90 TS 3.14–3.30 3.14–3.26 175–179 171–171 90 84 90 TSSCS 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90 MBD 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90	•	TSSCS	3.21-3.23	3.23-3.23	180-180	180-180	90	86	90
equat. api. equat. api. α β γ std. 3.26-3.30 3.25-3.25 176-178 177-177 90 86 90 86 90 D2 3.16-3.21 3.10-3.23 171-175 165-165 90 83 90 D3 3.20-3.26 3.14-3.23 174-180 173-173 90 84 90 D3BJ 3.18-3.23 3.13-3.19 174-179 173-173 90 84 90 TS 3.14-3.30 3.14-3.26 175-179 171-171 90 84 90 TSSCS 3.19-3.26 3.17-3.23 170-177 174-174 90 85 90 MBD 3.19-3.26 3.17-3.23 170-177 174-174 90 85 90		MBD	3.19-3.21	3.20-3.20	180-180	180-180	90	85	90
Std. 3.26-3.30 3.25-3.25 176-178 177-177 90 86 90 D2 3.16-3.21 3.10-3.23 171-175 165-165 90 83 90 D3 3.20-3.26 3.14-3.23 174-180 173-173 90 84 90 D3BJ 3.18-3.23 3.13-3.19 174-179 173-173 90 84 90 TS 3.14-3.30 3.14-3.26 175-179 171-171 90 84 90 TSSCS 3.19-3.26 3.17-3.23 170-177 174-174 90 85 90 MBD 3.19-3.26 3.17-3.23 170-177 174-174 90 85 90		dDsC	3.19–3.21	3.19–3.19	180–180	180–180	90	85	90
D2 3.16-3.21 3.10-3.23 171-175 165-165 90 83 90 D3 3.20-3.26 3.14-3.23 174-180 173-173 90 84 90 D3BJ 3.18-3.23 3.13-3.19 174-179 173-173 90 84 90 TS 3.14-3.30 3.14-3.26 175-179 171-171 90 84 90 TSSCS 3.19-3.26 3.17-3.23 170-177 174-174 90 85 90 MBD 3.19-3.26 3.17-3.23 170-177 174-174 90 85 90			equat.	api.	equat.	api.	α	β	γ
TSSCS 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90 MBD 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90	3	std.	3.26-3.30	3.25-3.25	176–178	177–177	90	86	90
TSSCS 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90 MBD 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90		D2	3.16-3.21	3.10-3.23	171–175	165–165	90	83	90
TSSCS 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90 MBD 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90	\mathbb{H}_3 F	D3	3.20-3.26	3.14-3.23	174–180	173–173	90	84	90
TSSCS 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90 MBD 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90	Sbl	D3BJ	3.18–3.23	3.13–3.19	174–179	173–173	90	84	90
TSSCS 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90 MBD 3.19–3.26 3.17–3.23 170–177 174–174 90 85 90	CH_{j}								
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dDsC 3.18–3.25 3.16–3.23 171–172 168–168 90 84 90		MBD	3.19-3.26	3.17-3.23	170–177	174–174	90	85	90
		dDsC	3.18–3.25	3.16–3.23	171–172	168–168	90	84	90

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