Supplementary Information
TcESTIME: Predicting high-temperature hydrogen-based superconductors

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November 7, 2024

Table 1: Effective radii, r_{eff} of the core of different chemical elements, as obtained from the atomic ELF in Kohout and Savin (1996).

Element	Z	r_{eff}
Li	3	1.53
Be	4	1.02
B	5	0.75
C	6	0.58
N	7	0.47
O	8	0.40
F	9	0.34
Ne	10	0.30
Na	11	2.135
Mg	12	1.686
Al	13	1.395
Si	14	1.183
P	15	1.024
S	16	0.912
Cl	17	0.817
Ar	18	0.739
K	19	3.07
Ca	20	2.55
Sc	21	2.39

Ti	22	2.29
V	23	2.20
Cr	24	2.37
Mn	25	2.07
Fe	26	2.01
Co	27	1.95
Ni	28	1.89
Cu	29	2.17
Zn	30	1.81
Ga	31	1.59
Ge	32	1.42
As	33	1.28
Se	34	1.18
Br	35	1.10
Kr	36	1.02
Rb	37	3.51
Sr	38	2.95
Cd	48	2.34

Table 2: List of binary hydrogen-based systems in the dataset, including their chemical formula, pressure (P), networking value ϕ, molecularity index ϕ^*, H_f, H_{DOS}, reference T_c, and reference from where it was taken.

Chem. form.	P (GPa)	ϕ	ϕ^*	H_f	H_{DOS}	T_c^{ref} (K)	Ref.
LiH_2	150	0.24	1.00	0.667	0.94924	0	
LiH_6	150	0.37	0.98	0.857	0.88063	38.34	
LiH_8	100	0.16	0.98	0.889	0.92588	31.04	
BeH_2	250	0.35	0.54	0.667	0.42005	44.1	
BeH_2	400	0.44	0.44	0.667	0.39974	62	
MgH_6	400	0.64	0.64	0.857	0.74105	271	
CaH_6	150	0.63	0.63	0.857	0.91338	235	
SrH_6	250	0.34	0.79	0.857	0.86045	156	
ScH_2	80	0.33	0.33	0.667	0.02726	32.9	
YH_4	120	0.44	0.6	0.800	0.39112	95	
YH_6	120	0.58	0.58	0.857	0.45269	264	
ScH_4	200	0.48	0.64	0.800	0.29856	98	
ScH_6	350	0.61	0.61	0.857	0.32246	169	
PrH_9	100	0.27	0.52	0.900	0.16150	0	
CeH_{10}	94	0.53	0.66	0.909	0.27900	168	
CeH_9	100	0.51	0.72	0.900	0.29135	50	
LaH_9	50	0.31	0.95	0.900	0.16123	30	

YH$_9$	150	0.58	0.79	0.900	0.65701	250
ScH$_9$	400	0.66	0.66	0.900	0.55013	180
YH$_{10}$	250	0.58	0.67	0.909	0.67017	326
LaH$_8$	300	0.0	0.75	0.889	0.38922	131
LaH$_{10}$	150	0.52	0.65	0.909	0.50395	274
ScH$_9$	300	0.59	0.94	0.900	0.53215	163
ScH$_{10}$	250	0.33	0.89	0.909	0.53668	120
ScH$_{12}$	350	0.33	0.86	0.923	0.58697	141
ScH$_7$	300	0.47	0.82	0.875	0.55962	169
ScH$_6$	130	0.26	0.88	0.857	0.42992	119
TiH$_2$	0	0.3	1.0	0.667	0.00053	7
TiH$_2$	0	0.18	0.4	0.667	0.03800	0
ZrH	120	0.33	0.33	0.500	0.01214	11
HfH$_2$	0	0.17	0.24	0.667	0.00787	0
HfH$_2$	180	0.23	0.78	0.667	0.11542	8
HfH$_2$	260	0.31	0.33	0.667	0.07105	12
NbH$_2$	60	0.29	0.4	0.667	0.00844	0.5
VH$_2$	0	0.31	0.31	0.667	0.00539	0.5
NbH$_2$	0	0.28	0.28	0.667	0.00668	1.5
NbH$_2$	60	0.35	0.39	0.667	0.01147	4
NbH$_4$	300	0.28	0.42	0.800	0.10784	47
TaH$_2$	200	0.41	0.43	0.667	0.03040	7.1
TaH$_4$	250	0.27	0.37	0.800	0.23240	31
TaH$_6$	300	0.4	0.61	0.857	0.48226	135.8
CrH	0	0.4	0.4	0.500	0.00636	10.6
CrH$_3$	81	0.38	0.38	0.750	0.07048	37.1
TcH$_3$	300	0.31	0.36	0.750	0.07314	9.94
FeH$_6$	150	0.36	1.0	0.857	0.18419	42.9
FeH$_5$	150	0.37	0.55	0.833	0.06091	45.8
RuH	100	0.28	0.28	0.500	0.01618	0.41
RuH$_3$	100	0.29	0.29	0.750	0.08244	3.57
RuH$_3$	200	0.29	0.29	0.750	0.13508	1.25
OsH	100	0.34	0.34	0.500	0.00788	2.1
CoH	5	0.27	0.27	0.500	0.00479	0.11
PdH	0	0.2	0.2	0.500	0.15803	9
PdH	0	0.2	0.2	0.500	0.15803	5
PtH	100	0.27	0.27	0.500	0.14640	15
PtH	80	0.28	0.32	0.500	0.08208	25
AuH	220	0.27	0.27	0.500	0.02230	21
BH	175	0.51	0.51	0.500	0.27223	21.4
BH$_3$	360	0.58	0.84	0.750	0.53550	125
AlH$_3$	73	0.41	0.41	0.750	0.67764	11.5
GaH$_3$	120	0.1	0.0	0.750	0.56491	102
InH$_5$	150	0.3	0.99	0.833	0.34432	27.1

InH$_3$	200	0.31	0.9	0.750	0.28419	40.5
SiH$_4$	125	0.48	0.81	0.800	0.59684	55
SiH$_4$	120	0.54	0.73	0.800	0.40524	74
SiH$_4$	400	0.47	0.57	0.800	0.54972	35
SiH$_4$	610	0.5	0.6	0.800	0.44245	110
SiH$_4$	300	0.48	0.98	0.800	0.25117	35.1
SiH$_4$	190	0.33	0.84	0.800	0.62307	16.5
Si$_2$H$_6$	200	0.48	0.77	0.750	0.35811	80
Si$_2$H$_6$	275	0.02	0.02	0.750	0.37144	153
Si$_2$H$_6$	300	0.54	0.96	0.750	0.35998	42
GeH$_4$	220	0.4	0.9	0.800	0.36688	64
GeH$_4$	250	0.31	0.95	0.800	0.41384	57
GeH$_4$	500	0.42	0.65	0.800	0.50236	84
GeH$_4$(H$_2$)2	250	0.35	0.93	0.889	0.52831	90
GeH$_4$	280	0.35	0.66	0.800	0.42974	67
Ge3H$_{11}$	285	0.33	0.42	0.786	0.47560	43
GeH$_3$	180	0.33	0.4	0.750	0.27853	90
GeH$_3$	180	0.32	0.35	0.750	0.24793	140
SnH$_8$	250	0.24	0.9	0.889	0.54617	72
SnH$_4$	120	0.23	0.98	0.800	0.30038	22
SnH$_4$	200	0.24	0.95	0.800	0.37070	62
SnH$_4$	600	0.29	0.93	0.800	0.38303	95
SnH$_{12}$	250	0.26	0.91	0.923	0.64144	93
SnH$_{14}$	300	0.37	0.96	0.933	0.71983	97
PbH$_4$(H$_2$)2	230	0.21	0.97	0.889	0.43717	107
PH$_4$	80	0.15	1.0	0.800	0.28436	1.9
PH$_2$	80	0.62	1.0	0.667	0.16935	29.5
AsH	300	0.45	0.45	0.500	0.16926	21.2
AsH$_8$	450	0.43	0.91	0.889	0.53430	151.4
SbH	175	0.37	0.39	0.500	0.13976	14.6
SbH$_4$	150	0.31	0.95	0.800	0.32348	102.2
BiH$_2$	125	0.33	0.97	0.667	0.19364	39
BiH$_3$	270	0.32	0.85	0.750	0.34636	65
SbH$_3$	170	0.35	0.91	0.750	0.27787	68
BiH	250	0.33	0.0	0.500	0.22987	30
BiH$_2$	300	0.32	0.94	0.667	0.21725	65
BiH$_4$	150	0.3	0.96	0.800	0.29603	93
BiH$_6$	300	0.29	0.85	0.857	0.46471	113
(H$_2$S)2H$_2$	200	0.69	0.69	0.750	0.47654	204
H$_3$S	150	0.71	0.71	0.750	0.48732	225
H$_4$S$_3$	140	0.38	0.77	0.571	0.22762	2.1
H$_5$S$_2$	130	0.28	0.89	0.714	0.40847	79
HSe$_2$	300	0.46	0.56	0.333	0.14294	5
HSe	300	0.53	0.0	0.500	0.14283	42

H_3Se	200	0.54	0.54	0.750	0.48394	116
HSe	300	0.52	0.55	0.500	0.15501	23
H_4Te	170	0.41	0.94	0.800	0.24914	104
H_5Te_2	200	0.37	0.86	0.714	0.25675	58
HTe	150	0.42	0.42	0.500	0.14264	28
H_4Te	270	0.36	0.92	0.800	0.28495	76
PoH_4	250	0.26	0.95	0.800	0.28468	53.6
PoH	300	0.0	0.31	0.500	0.20401	0.65
PoH_2	200	0.31	0.97	0.667	0.16772	0
PoH_6	200	0.34	0.97	0.857	0.32384	4.68
HBr	200	0.38	0.66	0.500	0.17697	51
HCl	360	0.49	0.68	0.500	0.17748	40
HBr	150	0.38	0.7	0.500	0.13735	27
HCl	250	0.39	0.76	0.500	0.13565	20
H_2I	100	0.12	0.99	0.667	0.09580	8
H_4I	300	0.25	0.95	0.800	0.31063	12.5
H_2I	100	0.0	0.99	0.667	0.11697	5.3
H_2I	240	0.27	0.94	0.667	0.16466	33
MgH_2	180	0.34	0.34	0.667	0.35378	23
MgH_4	100	0.27	1.0	0.800	0.66683	37
MgH_{12}	140	0.36	0.97	0.923	0.91945	60
PH_2	260	0.39	0.54	0.667	0.40477	95
H	500	0.64	0.64	1.00	1.00000	318
H	450	0.52	0.94	1.00	1.00000	109

Table 3: List of X-RE-H systems (X is s-block element, RE is rare earth.) in the dataset, including their chemical formula, pressure (P), networking value ϕ, molecularity index ϕ^*, H_f, H_{DOS}, reference T_c, and reference from where it was taken.

	P (GPa)	ϕ	ϕ^*	H_f	H_{DOS}	T_c^{ref} (K)	Ref.
$LiScH_{10}$	300	0.30	0.93	0.833	0.280	52	[1]
Li_2ScH_{20}	300	0.36	0.97	0.870	0.745	242	[1]
Li_2ScH_{16}	300	0.63	0.69	0.842	0.684	262	[1]
Li_2ScH_{16}	230	0.63	0.69	0.842	0.686	281	[1]
Li_2ScH_{17}	300	0.57	0.83	0.850	0.600	94	[1]
Li_2LaH_{17}	300	0.50	0.79	0.850	0.671	118	[1]
Li_2YH_{16}	300	0.59	0.71	0.842	0.769	251	[1]
Li_2YH_{17}	300	0.55	0.81	0.850	0.798	64	[1]
$CaYH_{20}$	600	0.54	0.70	0.909	0.819	250	[2]
Ca_2YH_{18}	200	0.58	0.67	0.857	0.752	217	[2]

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Ca_3YH_{24}	200	0.58	0.67	0.857	0.800	225	[2]
CaY_3H_{24}	200	0.55	0.63	0.857	0.558	252	[2]
$CaScH_2$	250	0.19	0.21	0.500	0.024	31	[3]
$CaScH_4$	200	0.17	0.49	0.667	0.098	2	[3]
$CaScH_6$	200	0.36	0.36	0.750	0.601	57	[3]
$CaScH_8$	200	0.42	0.88	0.800	0.557	212	[3]
$CaScH_{12}$	160	0.55	0.68	0.857	0.486	175	[3]
$BeLaH_8$	50	0.29	0.53	0.800	0.668	191	[4]
$BeYH_8$	100	0.12	0.36	0.800	0.697	249	[4]
$BeCeH_8$	30	0.29	0.52	0.800	0.779	201	[5]
$BeThH_7$	20	0.28	0.48	0.778	0.502	70	[5]
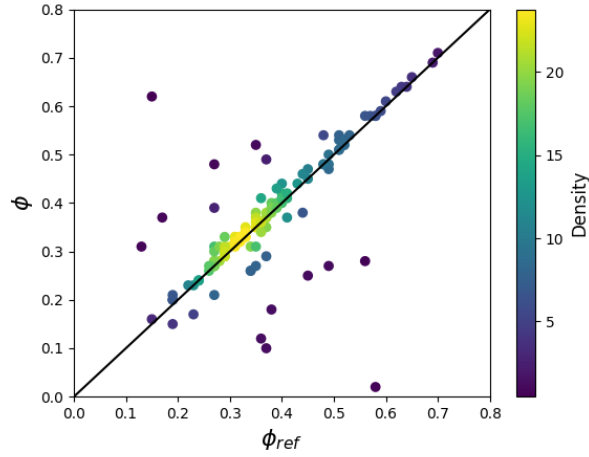
Figure 1: Values of ϕ computed with TcESTIME compared to the reference values, ϕ_{ref}, of the binary database. Colors represent the density of points per unit area.

Table 4: Prediction of the critical temperature of all binary and ternary compounds using four different fits, namely the least squares regression (LS), gradient boosting regression (GBR), and two different symbolic regression fits (SR2 and SR4). Reference T_c is provided for comparison.

Chem. form.	T_c	T_c^{LS}	T_c^{GBR}	T_c^{SR2}	T_c^{SR4}
LiH_2	0.00	62.33	-0.55	30.69	73.20
LiH_6	38.34	129.24	39.18	101.89	158.31
LiH_8	31.04	53.80	28.74	53.82	74.16

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BeH$_2$	44.10	70.32	49.54	68.90	71.01
BeH$_2$	62.00	89.20	105.68	82.98	87.09
MgH$_6$	271.00	217.04	275.09	239.65	251.20
CaH$_6$	235.00	229.59	241.77	266.06	274.52
SrH$_6$	156.00	117.01	148.54	142.03	143.80
ScH$_2$	32.90	20.77	24.50	21.67	17.06
YH$_4$	95.00	108.01	124.09	118.97	113.16
YH$_6$	264.00	164.71	210.94	187.31	177.93
ScH$_4$	98.00	107.66	105.95	103.94	107.85
ScH$_6$	169.00	154.13	117.39	158.09	157.94
PrH$_9$	0.00	50.93	11.00	97.18	53.24
CeH$_{10}$	168.00	134.20	163.88	152.66	139.43
CeH$_9$	50.00	129.40	126.46	137.49	135.08
LaH$_9$	30.00	59.84	53.60	46.61	61.08
YH$_9$	250.00	197.63	248.68	206.47	230.68
ScH$_9$	180.00	212.65	286.77	239.15	240.20
YH$_{10}$	326.00	201.08	240.50	247.48	236.49
LaH$_8$	131.00	-9.46	126.93	48.47	0.00
LaH$_{10}$	274.00	162.19	269.91	205.17	183.86
ScH$_9$	163.00	186.90	173.66	152.89	211.19
ScH$_{10}$	120.00	101.78	124.49	107.08	120.41
ScH$_{12}$	141.00	106.92	138.73	125.24	128.84
ScH$_7$	169.00	145.19	169.16	144.08	165.39
ScH$_6$	119.00	67.28	85.28	69.36	77.73
TiH$_2$	7.00	-2.07	13.07	0.91	2.16
TiH$_2$	0.00	8.96	-1.62	19.96	10.98
ZrH	11.00	7.85	15.85	6.09	7.39
HfH$_2$	0.00	0.83	17.82	10.83	4.72
HfH$_2$	8.00	24.63	7.15	20.07	24.46
HfH$_2$	12.00	29.62	8.26	34.28	25.87
NbH$_2$	0.50	8.51	3.26	10.73	8.34
VH$_2$	0.50	7.08	1.52	9.64	7.13
NbH$_2$	1.50	6.59	2.43	10.73	7.16
NbH$_2$	4.00	14.57	13.16	13.49	11.73
NbH$_4$	47.00	39.20	35.79	63.96	37.81
TaH$_2$	7.10	29.49	12.22	22.43	22.38
TaH$_4$	31.00	51.14	33.90	98.25	53.53
TaH$_6$	135.80	113.22	134.48	152.73	126.65
CrH	10.60	7.45	8.70	4.41	6.48
CrH$_3$	37.10	44.26	32.45	49.54	37.66
TcH$_3$	9.94	34.91	13.93	47.94	31.29
FeH$_6$	42.90	70.65	40.51	43.01	70.44
FeH$_5$	45.80	45.88	35.49	51.74	39.90
RuH	0.41	6.70	1.77	7.03	7.24

RuH$_3$	3.57	33.74	8.67	53.58	31.08
RuH$_3$	1.25	41.47	3.13	68.58	39.79
OsH	2.10	5.98	9.78	4.91	6.13
CoH	0.11	0.92	0.42	3.83	3.80
PdH	9.00	15.21	2.54	21.98	16.15
PdH	0.00	15.21	2.54	21.98	16.15
PtH	15.00	23.01	7.79	21.15	20.99
PtH	25.00	18.30	18.82	15.21	16.30
AuH	21.00	7.88	4.12	8.26	8.19
BH	21.40	65.96	57.01	28.85	54.07
BH$_3$	125.00	151.74	123.18	101.04	158.43
AlH$_3$	11.50	113.79	23.06	153.60	125.98
GaH$_3$	102.00	18.83	95.92	154.27	28.06
InH$_5$	27.10	70.47	27.85	46.50	76.92
InH$_3$	40.50	60.30	50.37	40.78	61.69
SiH$_4$	55.00	138.08	61.30	117.22	152.49
SiH$_4$	74.00	136.42	82.23	116.77	141.36
SiH$_4$	35.00	131.10	162.75	151.11	143.30
SiH$_4$	110.00	129.63	114.10	135.57	136.77
SiH$_4$	35.10	101.10	32.20	56.75	98.92
SiH$_4$	16.50	93.44	19.96	87.59	107.12
Si$_2$H$_6$	80.00	107.20	62.38	79.28	107.22
Si$_2$H$_6$	153.00	-4.54	77.76	113.72	4.55
Si$_2$H$_6$	42.00	122.01	46.71	64.93	120.94
GeH$_4$	64.00	95.08	68.35	68.58	99.63
GeH$_4$	57.00	74.88	76.71	52.45	82.01
GeH$_4$	84.00	112.43	177.65	123.59	122.41
GeH$_4$(H$_2$)2	90.00	105.33	86.36	94.87	122.55
GeH$_4$	67.00	86.96	74.25	102.43	94.35
Ge3H$_{11}$	43.00	82.93	87.13	134.79	91.14
GeH$_3$	90.00	64.30	81.29	91.58	65.01
GeH$_3$	140.00	59.34	45.16	90.12	59.48
SnH$_8$	72.00	70.13	76.62	78.08	85.44
SnH$_4$	22.00	46.77	17.72	31.03	51.84
SnH$_4$	62.00	53.48	26.61	39.98	60.09
SnH$_4$	95.00	67.43	72.92	50.46	73.81
SnH$_{12}$	93.00	84.99	89.44	97.49	106.12
SnH$_{14}$	97.00	131.72	102.66	124.96	162.58
PbH$_4$(H$_2$)2	107.00	55.20	35.90	49.31	66.89
PH$_4$	1.90	26.55	9.74	18.11	32.89
PH$_2$	29.50	94.95	36.60	33.49	79.88
AsH	21.20	47.34	12.84	22.75	37.62
AsH$_8$	151.40	132.09	161.71	118.12	151.41
SbH	14.60	34.35	13.74	20.26	28.11

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SbH$_4$	102.20	68.23	89.83	46.37	72.50
BiH$_2$	39.00	48.65	38.14	20.79	45.46
BiH$_3$	65.00	67.45	61.37	51.61	70.30
SbH$_3$	68.00	68.71	69.33	43.28	68.87
BiH	30.00	36.66	30.92	35.25	32.15
BiH$_2$	65.00	49.09	60.98	23.25	46.69
BiH$_4$	93.00	63.53	85.99	41.89	67.12
BiH$_6$	113.00	78.39	104.69	83.50	90.14
(H$_2$S)2H$_2$	204.00	175.00	201.05	128.81	177.80
H$_3$S	225.00	181.77	222.75	130.26	185.01
H$_4$S$_3$	2.10	51.00	13.24	23.96	44.96
H$_5$S$_2$	79.00	58.23	73.86	40.13	62.05
HSe$_2$	5.00	27.09	9.89	5.56	19.21
HSe	42.00	53.75	26.25	31.97	40.70
H$_3$Se	116.00	135.64	119.19	129.81	140.22
HSe	23.00	54.28	23.41	21.11	41.60
H$_4$Te	104.00	84.72	102.92	53.13	84.16
H$_5$Te$_2$	58.00	67.16	60.54	41.60	65.00
HTe	28.00	40.61	19.62	20.88	32.23
H$_4$Te	76.00	77.02	80.23	53.19	79.02
PoH$_4$	53.60	52.98	46.00	37.46	57.05
PoH	0.65	-9.46	5.75	17.23	0.00
PoH$_2$	0.00	42.58	3.21	18.28	39.75
PoH$_6$	4.68	81.85	14.01	58.62	88.22
HBr	51.00	39.22	49.92	16.75	32.48
HCl	40.00	53.37	51.68	18.87	41.94
HBr	27.00	35.28	24.38	13.93	28.62
HCl	20.00	36.26	18.56	12.83	29.19
H$_2$I	8.00	7.25	9.14	5.28	11.63
H$_4$I	12.50	52.35	25.24	37.86	57.30
H$_2$I	5.30	-9.46	8.43	0.45	0.00
H$_2$I	33.00	35.58	27.00	17.58	34.30
MgH$_2$	23.00	63.73	34.44	78.07	63.31
MgH$_4$	37.00	76.66	38.72	49.93	90.67
MgH$_{12}$	60.00	137.99	62.30	130.06	175.92
PH$_2$	95.00	78.35	84.15	70.98	77.68
H	318.00	282.60	257.96	442.30	367.81
H	109.00	227.84	108.06	256.53	298.84
LiScH$_{10}$	52.00	65.19	72.11	50.09	69.41
Li$_2$ScH$_{20}$	242.00	120.13	230.93	98.06	144.94
Li$_2$ScH$_{16}$	262.00	203.80	212.05	205.23	231.32
Li$_2$ScH$_{16}$	281.00	204.05	212.05	205.59	231.72
Li$_2$ScH$_{17}$	94.00	177.00	90.29	155.68	198.82
Li$_2$LaH$_{17}$	118.00	160.36	114.38	158.02	184.51

Li$_2$YH$_{16}$	251.00	198.25	239.15	203.78	229.76
Li$_2$YH$_{17}$	64.00	188.43	68.55	179.57	221.29
CaYH$_{20}$	250.00	200.09	229.74	252.49	243.36
Ca$_2$YH$_{18}$	217.00	196.80	230.89	219.67	229.30
Ca$_3$YH$_{24}$	225.00	201.11	221.84	226.59	236.53
CaY$_3$H$_{24}$	252.00	167.62	248.25	191.32	187.32
CaScH$_2$	31.00	2.99	2.63	8.34	5.94
CaScH$_4$	2.00	14.38	26.13	27.91	16.64
CaScH$_6$	57.00	94.54	75.24	144.70	104.21
CaScH$_8$	212.00	116.69	201.36	91.26	128.89
CaScH$_{12}$	175.00	159.67	203.13	168.88	174.85
BeLaH$_8$	191.00	83.08	111.63	140.65	97.45
BeYH$_8$	249.00	29.38	242.54	143.70	41.20
BeCeH$_8$	201.00	87.94	197.01	153.86	105.23
BeThH$_7$	70.00	69.53	78.12	118.03	78.22
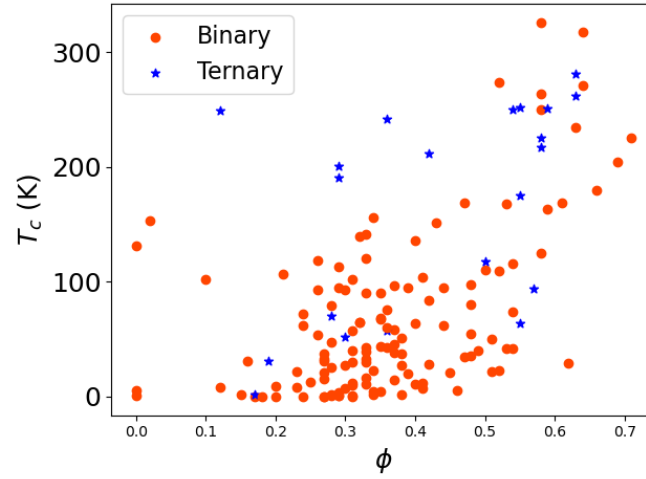
Figure 2: Reference T_c values with respect to the networking value, ϕ, of the binary and ternary systems in the database.
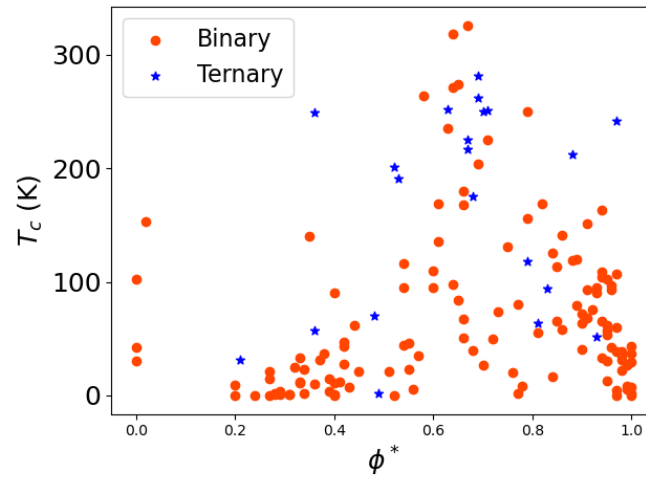

Figure 3: Reference T_c values with respect to the molecularity index, ϕ^*, of the binary and ternary systems in the database.
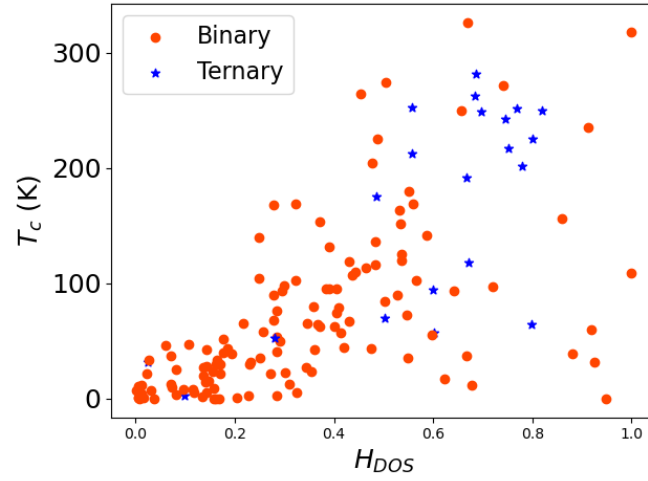
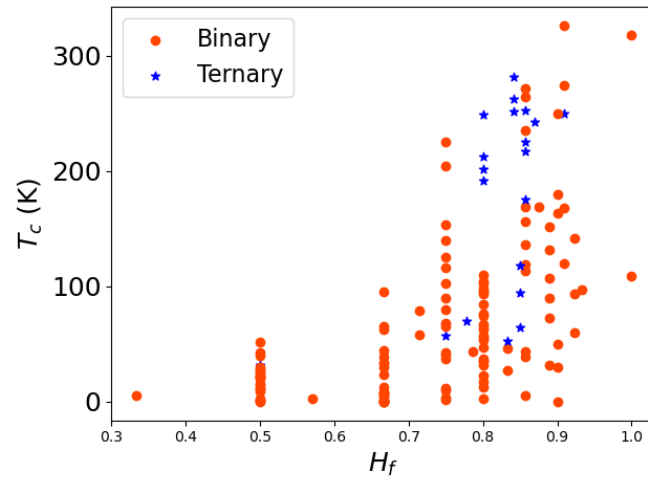Figure 4: Reference T_c values with respect to H_{DOS} of the binary and ternary systems in the database.

Figure 5: Reference T_c values with respect to the hydrogen fraction, H_f, of the binary and ternary systems in the database.

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