A simple semiempirical method for predicting the temperature-entropy saturation curve of pure fluids

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Supporting Information

Table S1

Table S1: Critical temperature T_{c}, acentric factor ω, maximum slope ξ^*_{M}, reduced temperature at point M T_{Mr}, intermolecular separation at zero potential energy σ_{c}, and percent relative deviations Δ_{r1} and Δ_{r2} . The fluids are listed in increasing value of ξ^*_{M}.

Fluid	T_{c}/K	ω	ξ^*_{M}	T_{Mr}	σ_{c}/nm	Δ_{r1} (%)	Δ_{r2} (%)
methanol	513.38	0.5625	−10.6364	0.7874	0.3913	7.74	12.4
heavy water	643.85	0.364	−9.877	0.8071	0.3094	2.86	10.35
water	647.1	0.3443	−9.846	0.8018	0.3088	2.96	11.7
ammonia	405.4	0.256	−8.6109	0.8162	0.3415	4.82	3.69
hydrogen chloride	324.55	0.1288	−8.3196	0.8228	0.3601	7.06	6.08
R41	317.28	0.2004	−7.9926	0.8146	0.384	4.02	4.02
carbon dioxide	304.13	0.2239	−7.9381	0.8219	0.3673	4.71	5.12
R32	351.26	0.2769	−7.7684	0.8198	0.4012	3.34	5.01
xenon	289.73	0.0036	−7.6918	0.8142	0.3972	3.95	3.4
krypton	209.48	−0.0009	−7.6578	0.8124	0.3647	4.31	7.97

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Table S1 – continued from previous page

Fluid	T_c/K	ω	ξ_M^*	T_{Mr}	σ_c/nm	Δ_{r1} (%)	Δ_{r2} (%)
argon	150.69	−0.0022	−7.6561	0.8117	0.3399	2.99	8.91
neon	44.49	−0.0387	−7.3103	0.8012	0.2804	4.27	2.73
sulfur dioxide	430.64	0.2557	−7.2518	0.8202	0.4005	3.64	1.26
nitrous oxide	309.52	0.162	−7.0185	0.8224	0.3715	4.23	10.06
R23	299.29	0.263	−6.8638	0.8205	0.4121	3.13	2.56
carbon monoxide	132.86	0.0497	−6.8622	0.8091	0.3647	3.61	13.02
fluorine	144.41	0.0449	−6.8234	0.8118	0.3231	1.54	11.26
nitrogen	126.19	0.0372	−6.8113	0.806	0.3611	2.61	13.28
hydrogen sulfide	373.1	0.1005	−6.8028	0.8072	0.3724	3.59	11.69
oxygen	154.58	0.0222	−6.72	0.8054	0.338	3.77	17.0
ethylene	282.35	0.0866	−6.1541	0.8156	0.41	3.39	4.56
deuterium	38.34	−0.136	−6.0597	0.7992	0.3126	3.7	22.01
R40	416.3	0.243	−6.0057	0.8311	0.4183	12.65	12.62
methane	190.56	0.0114	−5.9212	0.7978	0.3731	1.57	17.05
nitrogen trifluoride	234.0	0.126	−5.8855	0.8261	0.4051	6.46	11.09
R14	227.51	0.1785	−5.7507	0.8153	0.4199	2.73	2.48
orthohydrogen	33.22	−0.218	−5.5374	0.7814	0.3242	4.27	33.94
carbonyl sulfide	378.77	0.0978	−5.4797	0.8131	0.4142	1.53	5.78
ethanol	514.71	0.646	−5.4382	0.8407	0.4461	1.56	7.08
parahydrogen	32.94	−0.219	−5.4225	0.7856	0.3236	4.84	33.18
hydrogen	33.15	−0.219	−5.3996	0.7873	0.3238	4.94	33.42
ethane	305.32	0.0995	−4.838	0.8145	0.425	2.68	6.46
R22	369.3	0.2208	−4.8229	0.819	0.4429	3.47	2.47
R161	375.25	0.216	−4.4255	0.8205	0.4376	2.05	1.98
propyne	402.38	0.204	−3.5995	0.7971	0.4416	4.22	7.49
helium	5.2	−0.385	−3.5483	0.7489	0.3117	13.86	69.56
R152a	386.41	0.2752	−3.4813	0.8223	0.4555	2.6	2.28
R13	302.0	0.1723	−3.3923	0.8226	0.4552	2.73	1.86
cyclopropane	398.3	0.1305	−2.9929	0.8469	0.4409	7.88	15.33
R21	451.48	0.2061	−2.9492	0.818	0.4688	4.12	5.16
propylene	364.21	0.146	−2.7352	0.8214	0.4586	3.39	2.41
R143a	345.86	0.2615	−2.4733	0.8183	0.4682	2.09	3.77
DME	400.38	0.196	−2.4475	0.8198	0.4458	3.03	11.29
trifluoroiodomethane	396.44	0.176	−2.4241	0.7992	0.4916	1.1	21.92
R134a	374.21	0.3268	−1.5632	0.8172	0.4717	2.73	1.22
R12	385.12	0.1795	−1.508	0.8043	0.483	1.23	8.0
propane	369.89	0.1521	−1.3906	0.8214	0.4722	3.39	2.31
R125	339.17	0.3052	−0.5398	0.8089	0.4794	2.0	1.78
acetone	508.1	0.3071	−0.3538	0.8173	0.482	4.12	4.12
RE143a	377.92	0.289	−0.1089	0.818	0.4838	1.71	1.47
sulfur hexafluoride	318.72	0.21	−0.0175	0.8201	0.4696	3.52	11.67
R142b	410.26	0.2321	0.1386	0.8155	0.4913	2.49	2.96
R11	471.11	0.1888	0.234	0.7864	0.5073	1.53	14.7

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Fluid	T_c/K	ω	ξ_M^*	T_{Mr}	σ_c/nm	Δ_{r1} (%)	Δ_{r2} (%)
R116	293.03	0.2566	0.4458	0.8128	0.4911	2.89	1.36
cis-butene	435.75	0.202	0.9697	0.8248	0.4987	4.54	2.66
R1234ze	382.51	0.313	1.0989	0.8034	0.4969	1.25	1.69
1-butene	419.29	0.192	1.3717	0.823	0.4989	3.11	1.61
R1234yf	367.85	0.276	1.3815	0.8076	0.5016	1.1	3.91
R124	395.42	0.2881	1.5614	0.8091	0.5043	2.17	3.73
trans-butene	428.61	0.21	1.6935	0.8185	0.4999	2.07	1.31
isobutene	418.09	0.193	1.8248	0.8193	0.5016	4.27	1.94
R141b	477.5	0.2195	2.3839	0.8112	0.512	1.87	5.62
R115	353.1	0.248	2.9004	0.8079	0.5095	1.01	2.03
isobutane	407.81	0.184	3.044	0.8223	0.5138	3.54	2.61
R1233zd	438.75	0.305	3.0552	0.7975	0.5235	1.27	10.97
R123	456.83	0.2819	3.4213	0.7994	0.527	1.04	11.94
butane	425.12	0.201	3.5432	0.8181	0.512	3.05	2.86
R1216	358.9	0.333	3.6838	0.8095	0.5135	0.8	0.91
R245fa	427.16	0.3776	4.1683	0.8193	0.5152	2.73	3.48
R236fa	398.07	0.377	4.6989	0.7995	0.5256	1.28	3.68
R114	418.83	0.2523	5.4626	0.7781	0.5373	1.94	8.46
cyclopentane	511.72	0.201	5.524	0.8268	0.5165	5.52	13.77
R236ea	412.44	0.369	5.7807	0.7922	0.5213	1.51	5.21
R245ca	447.57	0.355	5.9462	0.8074	0.5121	1.41	12.96
R227ea	374.9	0.357	6.0234	0.8071	0.5321	1.48	1.09
benzene	562.02	0.211	6.1558	0.8252	0.5129	2.11	17.11
RE245cb2	406.81	0.354	7.0324	0.796	0.5408	1.39	3.9
DEE	466.7	0.281	7.039	0.8045	0.5287	3.34	10.01
R218	345.02	0.3172	7.2705	0.8054	0.5402	1.59	1.24
DMC	557.0	0.346	7.3867	0.8129	0.5087	2.91	20.62
R113	487.21	0.2525	7.4017	0.7761	0.5605	2.43	21.28
RE245fa2	444.88	0.387	7.9754	0.7977	0.5353	1.67	7.72
neopentane	433.74	0.1961	8.1324	0.8216	0.544	2.49	1.47
isopentane	460.35	0.2274	8.3612	0.8179	0.5439	1.81	2.18
pentane	469.7	0.251	8.4366	0.816	0.547	1.33	1.27
RC318	388.38	0.3553	9.8443	0.7961	0.5538	1.76	1.97
R365mfc	460.0	0.377	10.1649	0.8151	0.5479	1.28	5.84
toluene	591.75	0.2657	10.8934	0.8121	0.5497	1.61	11.35
cyclohexane	553.6	0.2096	12.5657	0.8378	0.5466	5.14	28.69
hexane	507.82	0.299	13.6814	0.8127	0.5794	1.87	3.03
isohexane	497.7	0.2797	13.7711	0.8125	0.5788	3.02	1.37
RE347mcc	437.7	0.403	14.2038	0.7903	0.5857	2.02	6.77
perfluorobutane	386.33	0.371	14.8856	0.7876	0.5933	1.76	10.76
m-xylene	616.89	0.326	16.0966	0.8077	0.5824	0.7	6.78
p-xylene	616.17	0.324	16.0973	0.8127	0.5803	1.82	7.92
ethylbenzene	617.12	0.305	16.926	0.8164	0.5769	1.03	15.99

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Table S1 – continued from previous page

Fluid	T_c/K	ω	ξ_M^*	T_{Mr}	σ_c/nm	Δ_{r1} (%)	Δ_{r2} (%)
o-xylene	630.26	0.312	17.4037	0.8105	0.581	2.15	16.91
methylcyclohexane	572.2	0.234	18.5937	0.8222	0.5784	4.93	31.05
heptane	540.13	0.349	19.2387	0.8059	0.6103	3.71	4.21
perfluoropentane	420.56	0.423	22.8082	0.7793	0.6289	3.7	6.44
octane	569.32	0.395	25.1117	0.8011	0.6349	1.37	3.24
isooctane	544.0	0.303	25.2627	0.8145	0.6285	1.38	6.06
novec649	441.81	0.471	28.6415	0.7003	0.6496	18.68	10.33
MM	518.7	0.418	28.6999	0.7645	0.6548	13.84	19.76
nonane	594.55	0.4433	31.1834	0.7963	0.6625	2.59	7.56
propylcyclohhexane	630.8	0.326	31.4514	0.8077	0.6346	3.26	34.6
decane	617.7	0.4884	37.192	0.7864	0.6847	5.94	8.29
undecane	638.8	0.539	43.7309	0.7863	0.703	6.12	3.09
MDM	564.09	0.529	48.9411	0.7539	0.7857	8.89	89.22
dodecane	658.1	0.574	50.0562	0.7743	0.7342	5.8	10.92
D4	586.49	0.592	52.9243	0.7727	0.7982	6.19	83.57
MD2M	599.4	0.668	66.2116	0.7353	0.8318	20.4	85.78
D5	619.23	0.658	73.8466	0.7473	0.8738	11.98	111.06
methyl palmitate	755.0	0.91	86.6279	0.7388	0.8372	24.68	15.13
methyl linolenate	772.0	1.14	87.0511	0.7625	0.8533	17.94	28.42
MD3M	628.36	0.722	92.3726	0.7165	0.9156	23.44	106.31
methyl linoleate	799.0	0.805	96.4907	0.7361	0.8668	14.41	8.77
methyl oleate	782.0	0.906	97.9157	0.7395	0.8652	24.02	11.55
methyl stearate	775.0	1.02	100.2849	0.7366	0.8719	27.94	15.94
D6	645.78	0.736	104.5704	0.6897	0.9432	34.1	109.64
MD4M	653.2	0.825	106.7797	0.7384	0.9457	21.34	95.1

Table S2

The liquid-vapor saturation curve in a $T_{\mathrm{r}} - s^*$ diagram for the 121 pure fluids included in the RefProp 9.1 program.[1] The label for each plot includes: the RefProp 9.1 fluid number, the RefProp 9.1 short name of the fluid, the acentric factor ω, and the value of ξ^*_{M} reported in Table S1. The fluids are ordered in increasing value of ξ^*_{M}. The lines are the results of approximation A1: $s^*_{\mathrm{l,A1}}$ (dashed blue lines), $s^*_{\mathrm{g,A1}}$ (red lines), and $s^*_{0.385,\mathrm{A1}}$ (dotted lines), obtained from eqs 9, 8, and 5 of the main text, respectively, with the parameter a given by eq 13 (see main text). The symbols are the RefProp 9.1[1] results $s^*_{\mathrm{l,RP}}$ (triangles), $s^*_{\mathrm{g,RP}}$ (circles), and $s^*_{0.385,\mathrm{RP}}$ (squares). $s^*_{0.385,\mathrm{RP}}$ has been obtained from eq 1 of the main text. This Table should be considered as an extension of the results presented in Figure 2 of the main text.

Table S2

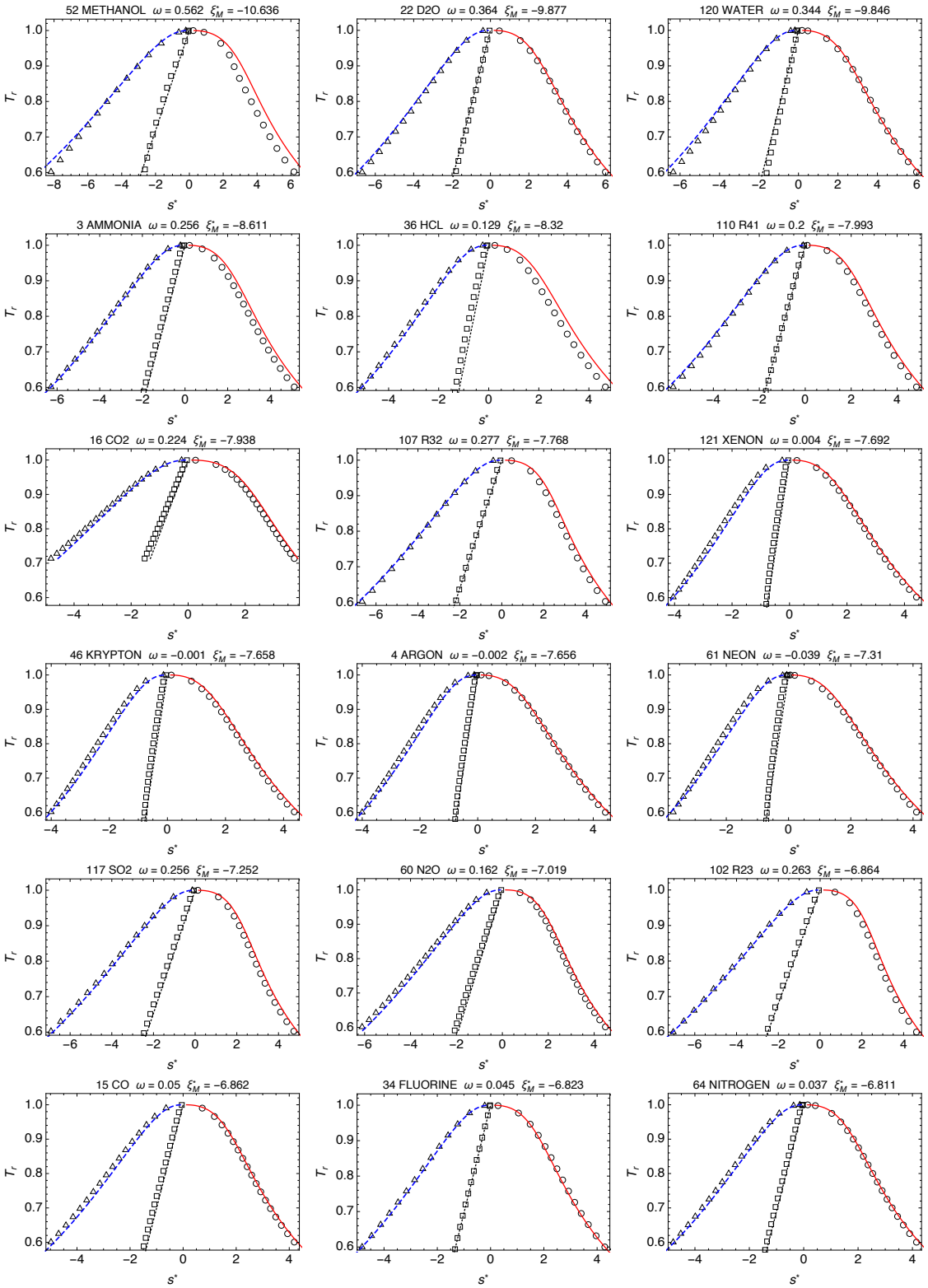
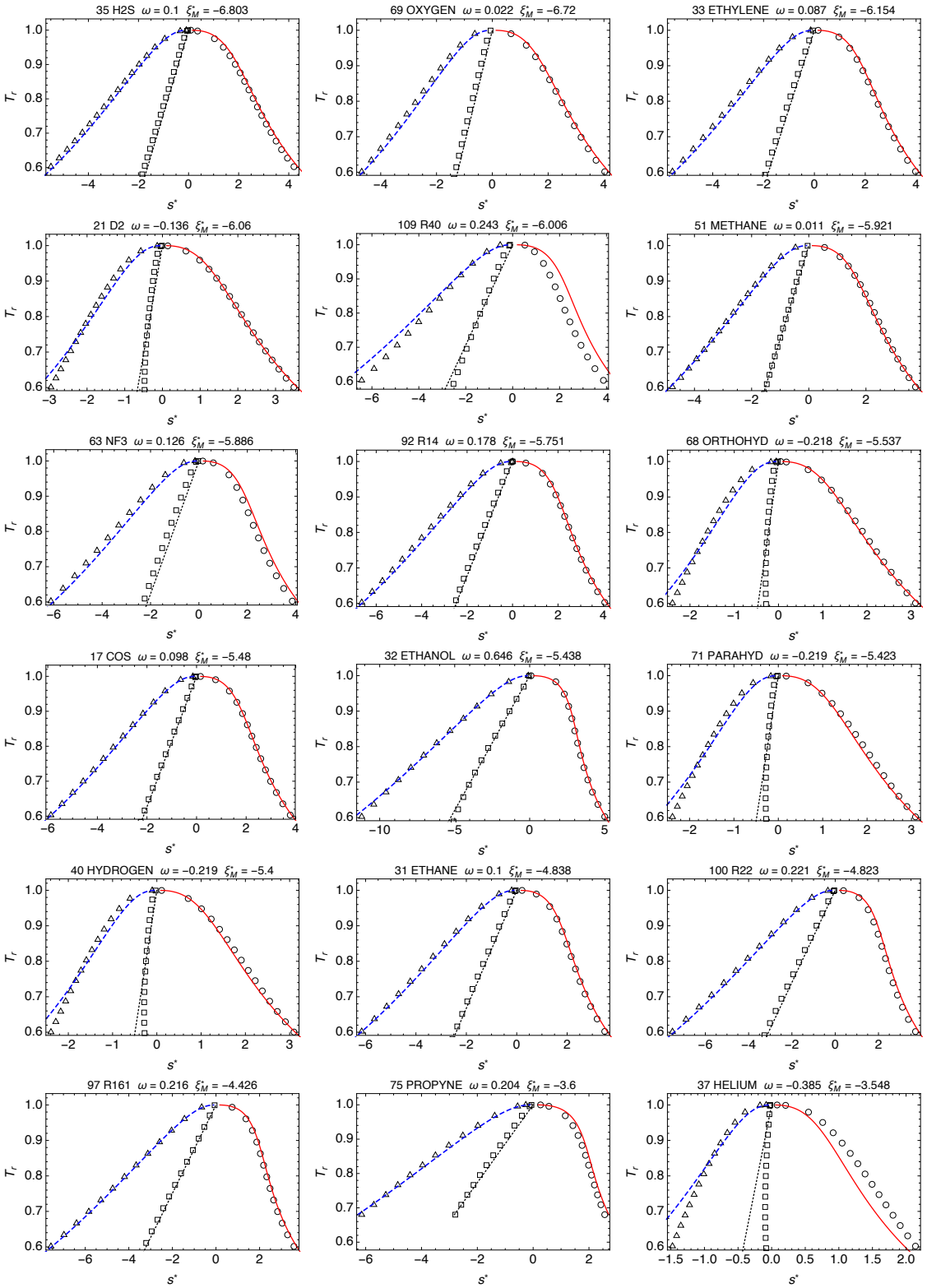

52 METHANOL ω = 0.562 ξ*M = −10.636
22 D2O ω = 0.364 ξ*M = −9.877
120 WATER ω = 0.344 ξ*M = −9.846
3 AMMONIA ω = 0.256 ξ*M = −8.611
36 HCL ω = 0.129 ξ*M = −8.32
110 R41 ω = 0.2 ξ*M = −7.993
16 CO2 ω = 0.224 ξ*M = −7.938
107 R32 ω = 0.277 ξ*M = −7.768
121 XENON ω = 0.004 ξ*M = −7.692
46 KRYPTON ω = −0.001 ξ*M = −7.658
4 ARGON ω = −0.002 ξ*M = −7.656
61 NEON ω = −0.039 ξ*M = −7.31
117 SO2 ω = 0.256 ξ*M = −7.252
60 N2O ω = 0.162 ξ*M = −7.019
102 R23 ω = 0.263 ξ*M = −6.864
15 CO ω = 0.05 ξ*M = −6.862
34 FLUORINE ω = 0.045 ξ*M = −6.823
64 NITROGEN ω = 0.037 ξ*M = −6.811
Tr
s*

Table S2 (*continued*)



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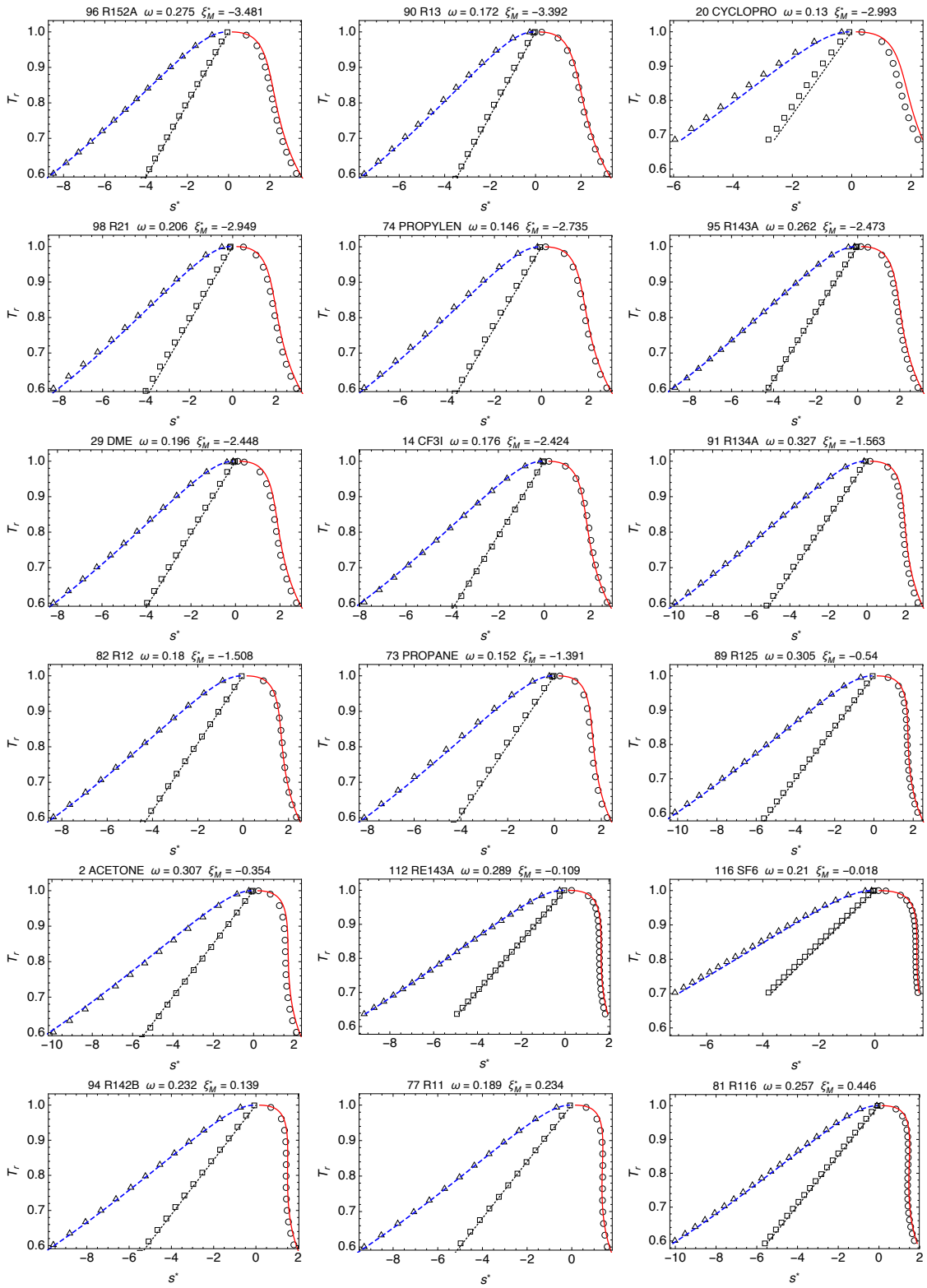

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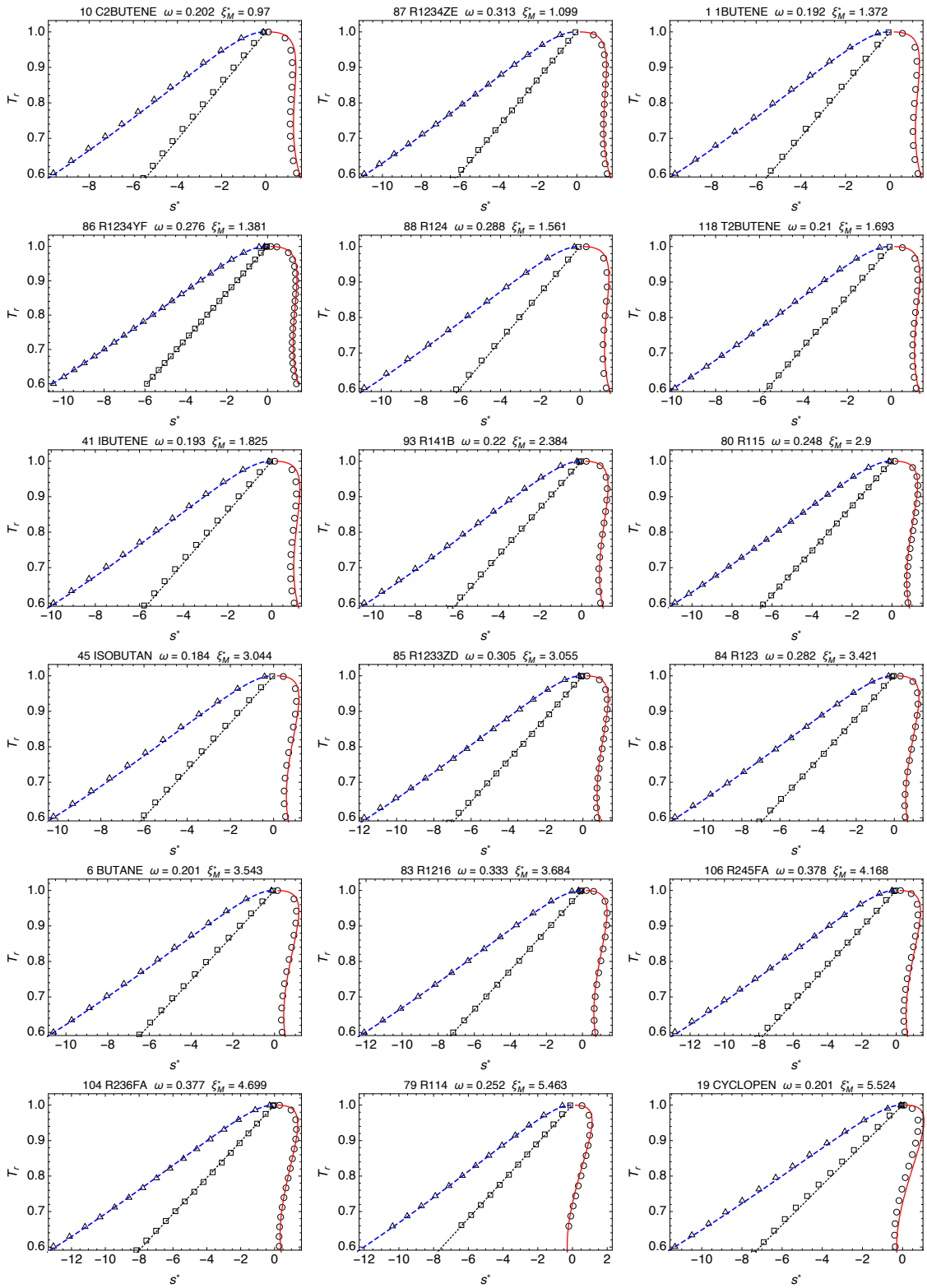

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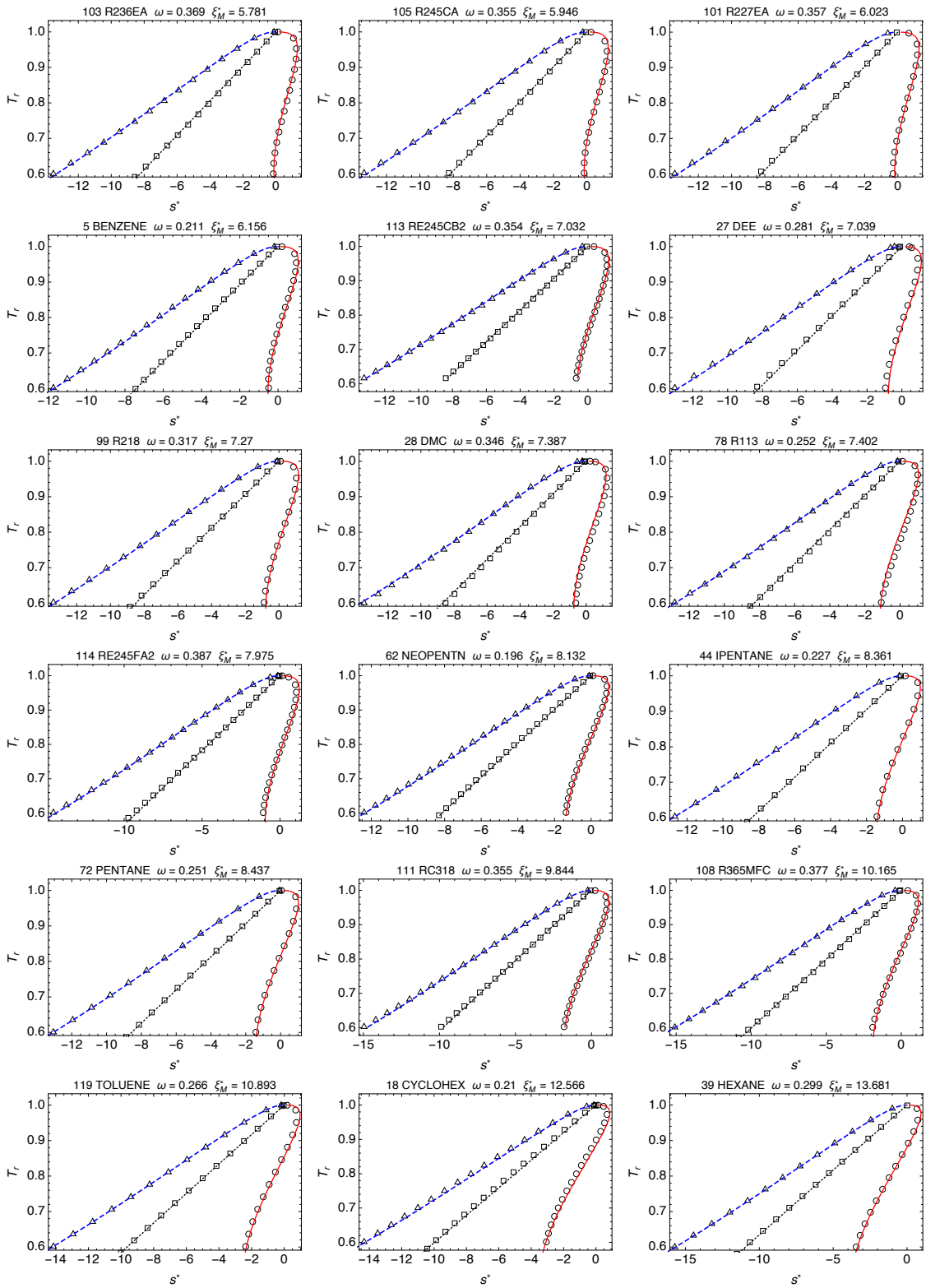

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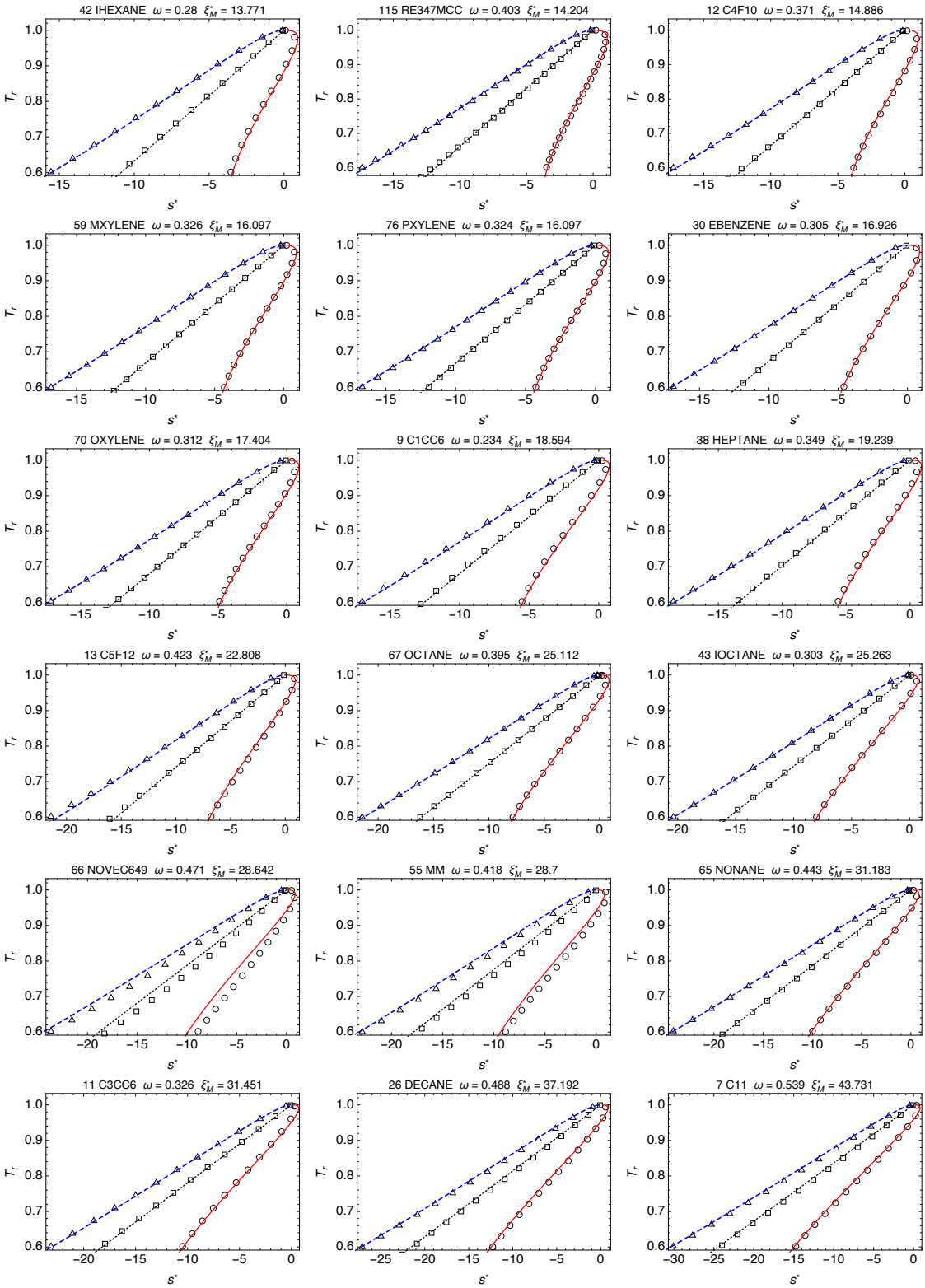

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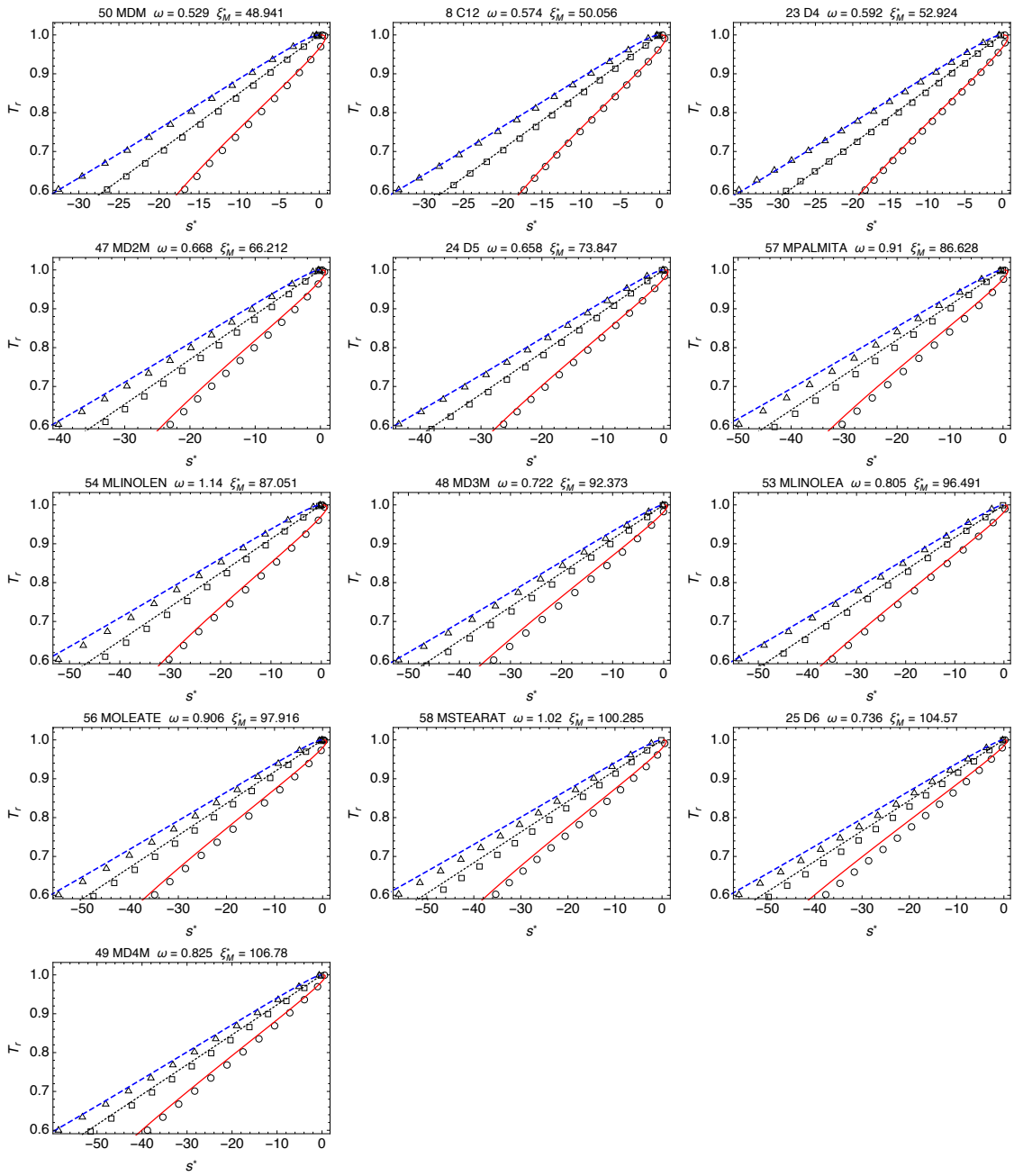


Table S3

The liquid-vapor saturation curve in a $T_\mathrm{r} - s^*$ diagram for the 121 pure fluids included in the RefProp 9.1 program.[1] The label for each plot includes: the RefProp 9.1 fluid number, the RefProp 9.1 short name of the fluid, the acentric factor ω, and the intermolecular separation at zero potential energy σ_c reported in Table S1. Like in Table S2, the fluids are ordered in increasing value of ξ^*_M. The lines are the results of approximation A2: $s^*_\mathrm{l,A2}$ (dashed blue lines), $s^*_\mathrm{g,A2}$ (red lines), and $s^*_\mathrm{0.385,A2}$ (dotted lines), obtained from eqs 9, 8, and 5 of the main text, respectively, with the parameter a given by equation 15 of the main text. The symbols are the RefProp 9.1[1] results $s^*_\mathrm{l,RP}$ (triangles), $s^*_\mathrm{g,RP}$ (circles), and $s^*_\mathrm{0.385,RP}$ (squares). $s^*_\mathrm{0.385,RP}$ has been obtained from eq 1 of the main text. This Table should be considered as an extension of the results presented in Figure 3 of the main text.

Table S3

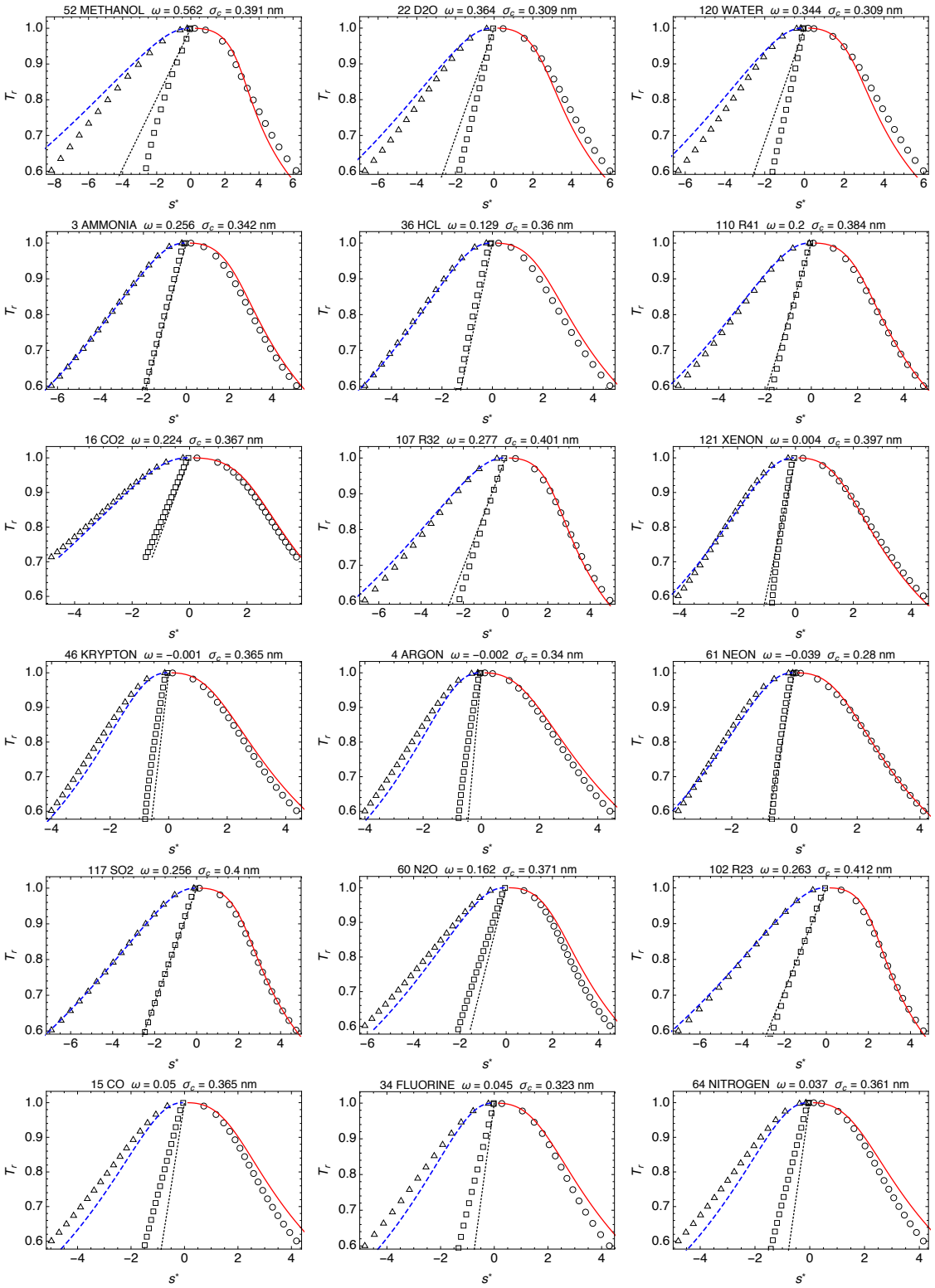
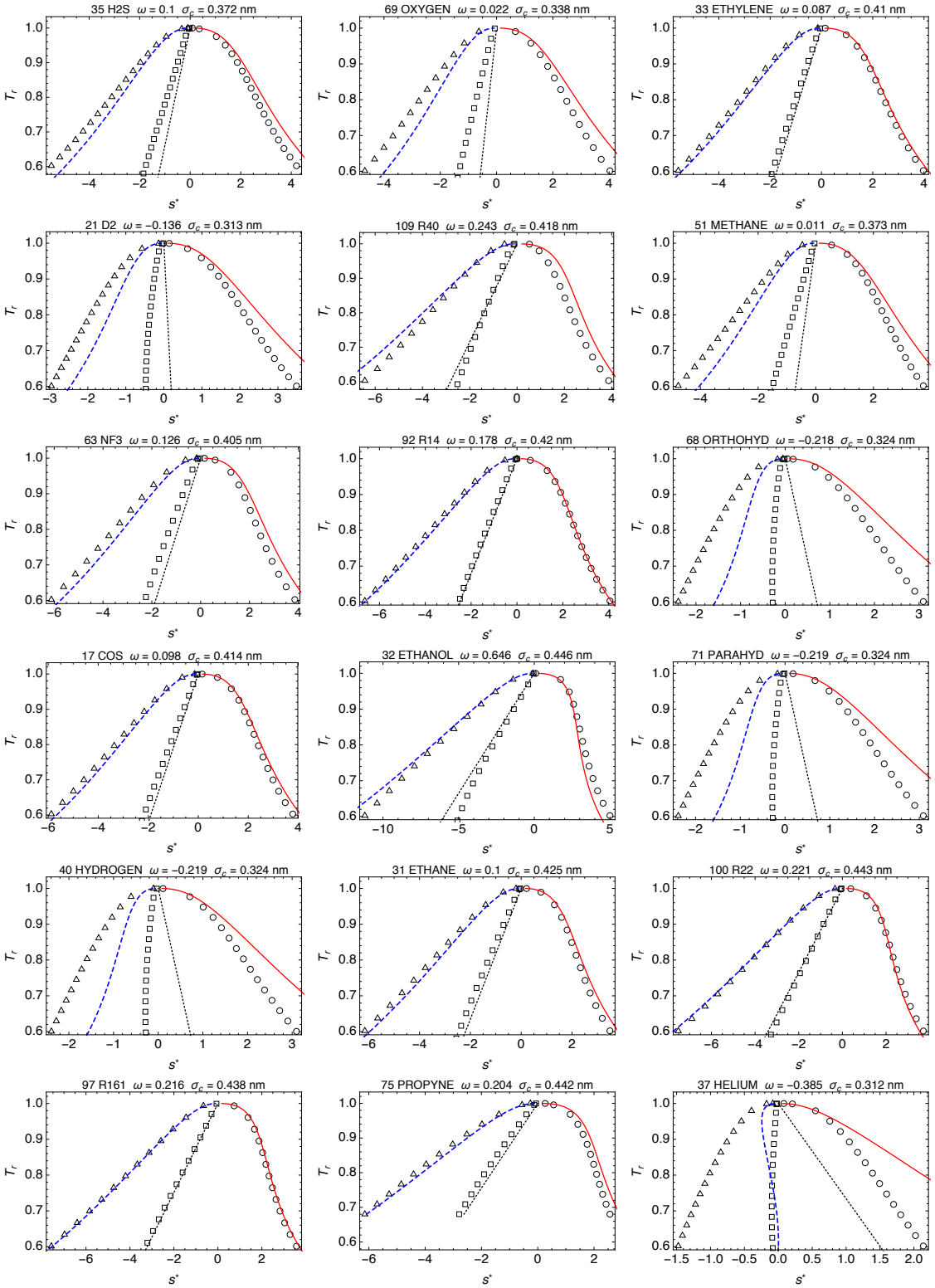

52 METHANOL ω = 0.562 σc = 0.391 nm
22 D2O ω = 0.364 σc = 0.309 nm
120 WATER ω = 0.344 σc = 0.309 nm
3 AMMONIA ω = 0.256 σc = 0.342 nm
36 HCL ω = 0.129 σc = 0.36 nm
110 R41 ω = 0.2 σc = 0.384 nm
16 CO2 ω = 0.224 σc = 0.367 nm
107 R32 ω = 0.277 σc = 0.401 nm
121 XENON ω = 0.004 σc = 0.397 nm
46 KRYPTON ω = −0.001 σc = 0.365 nm
4 ARGON ω = −0.002 σc = 0.34 nm
61 NEON ω = −0.039 σc = 0.28 nm
117 SO2 ω = 0.256 σc = 0.4 nm
60 N2O ω = 0.162 σc = 0.371 nm
102 R23 ω = 0.263 σc = 0.412 nm
15 CO ω = 0.05 σc = 0.365 nm
34 FLUORINE ω = 0.045 σc = 0.323 nm
64 NITROGEN ω = 0.037 σc = 0.361 nm
Tr
s*

Table S3 (*continued*)



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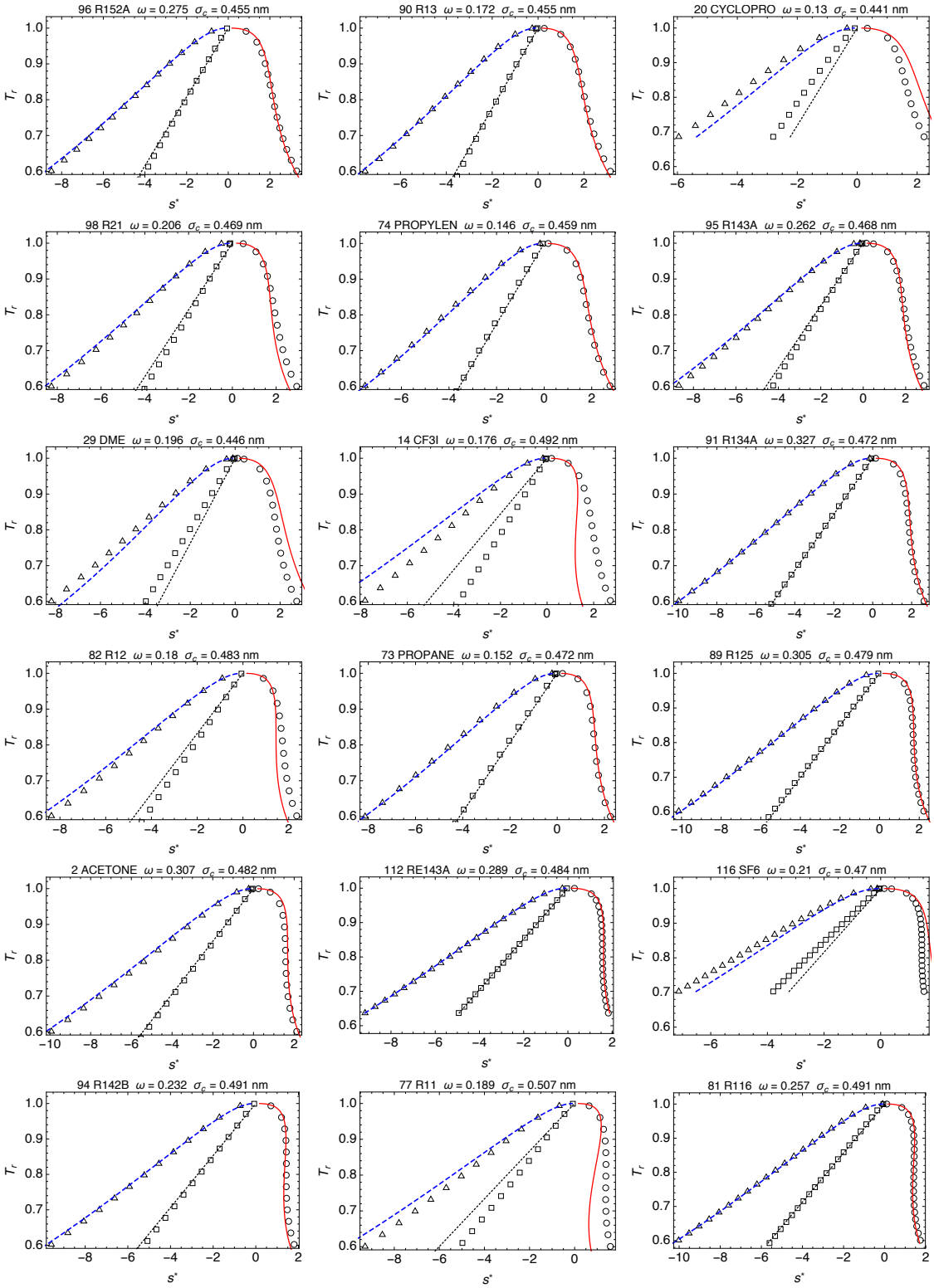

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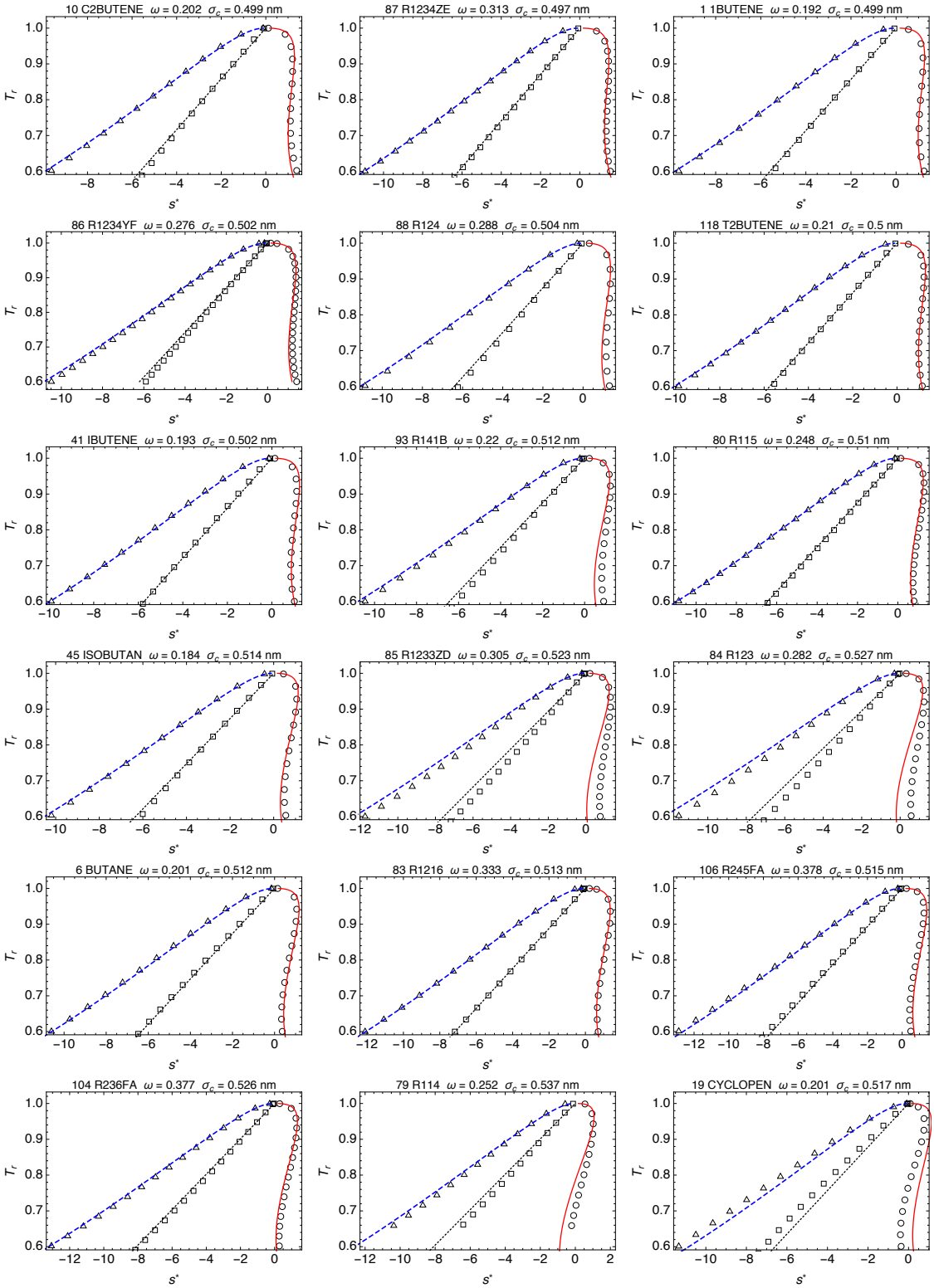

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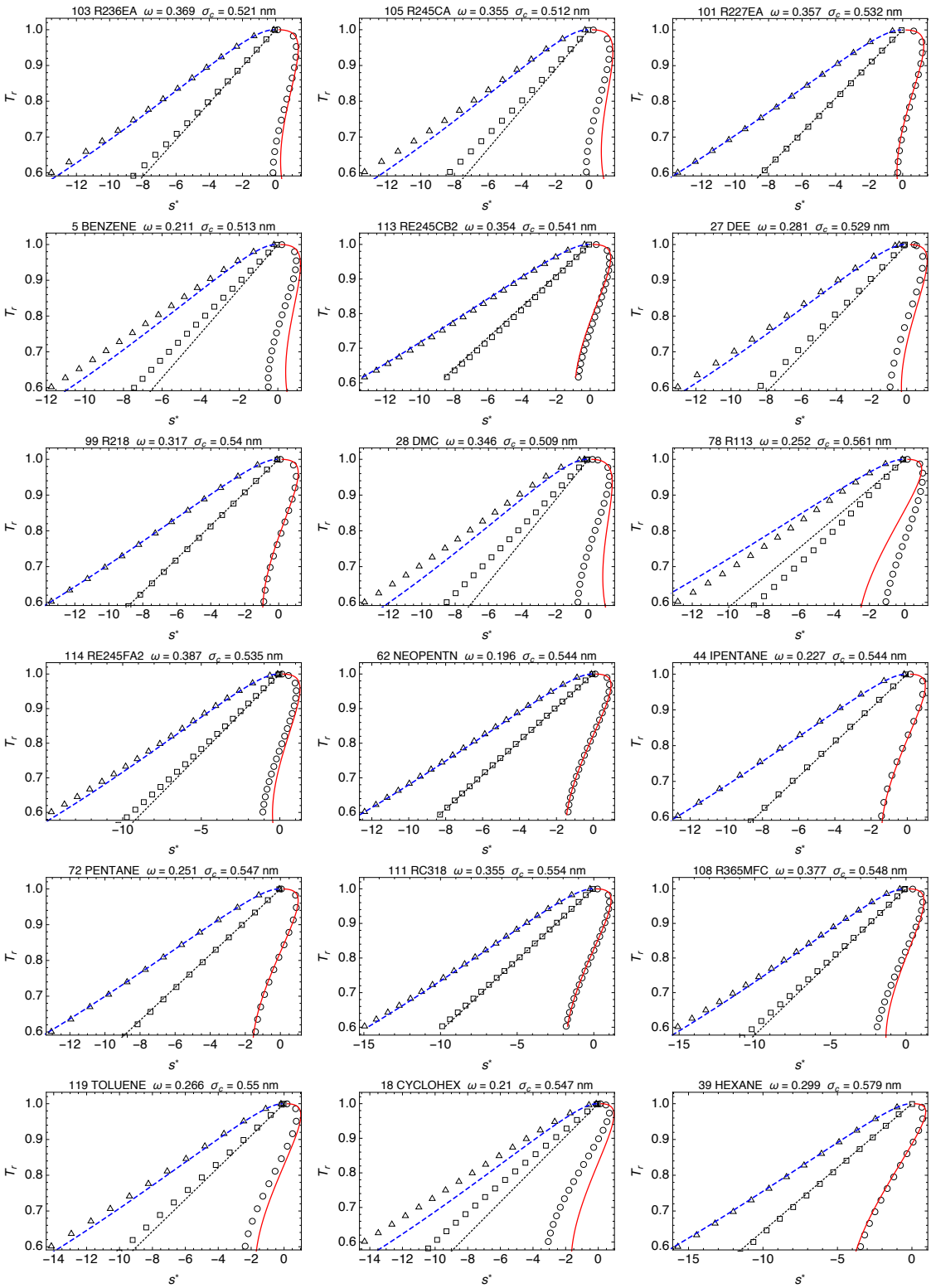

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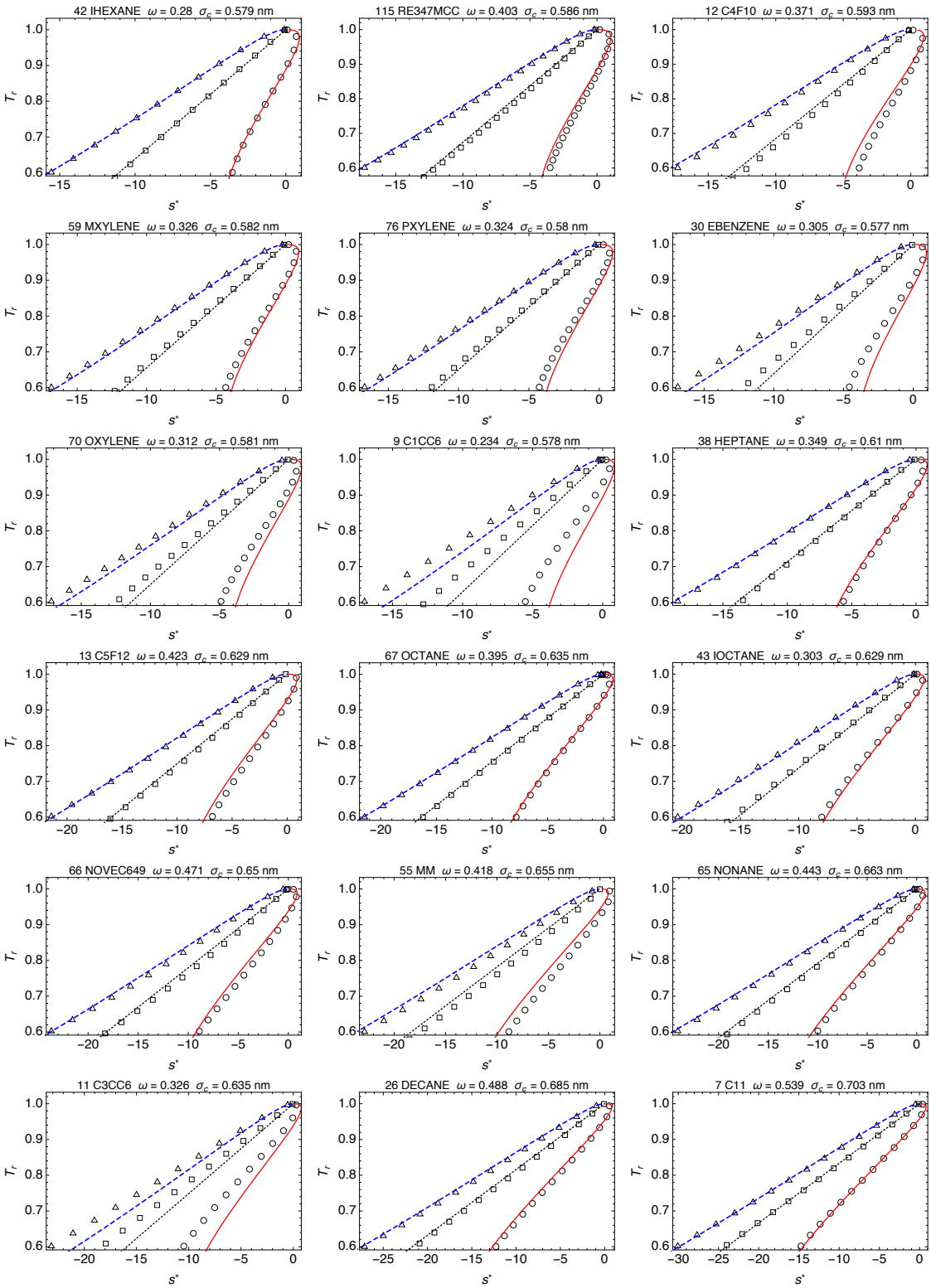

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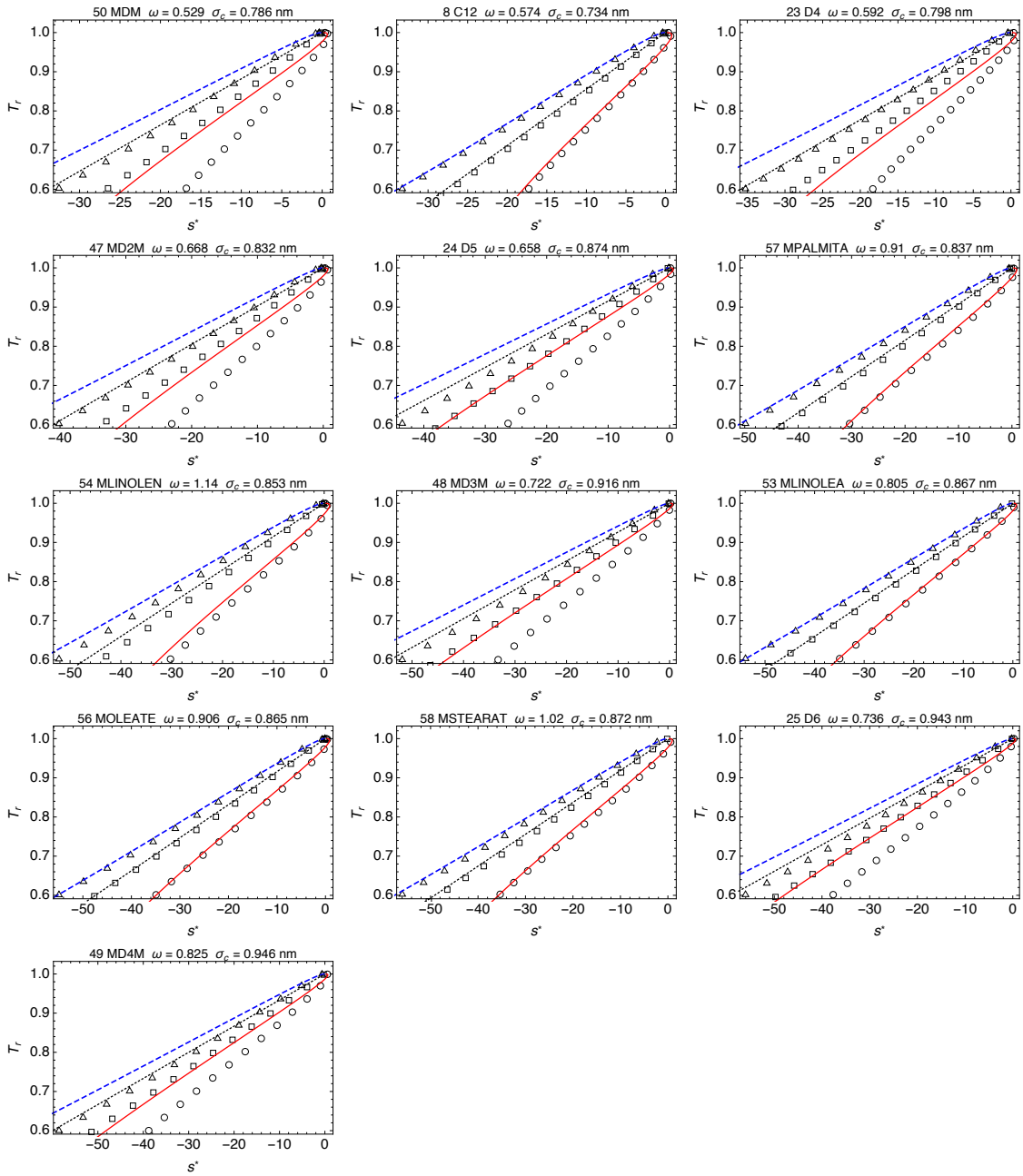

Acknowledgement

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References

(1) Lemmon, E. W.; Huber, M. L.; McLinden, M. O. NIST Standard Reference Database 23: Reference Fluid Thermodynamic and Transport Properties-REFPROP, Version 9.1. National Institute of Standards and Technology, Standard Reference Data Program, Gaithersburg, 2013.