Electronic Supplementary Information for: Capping the calix: solvation and recognition of Cs(I) through cation-pi interactions

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ESI1: EXAFS Collection and Analysis of Cs-C4P-Br Solution in Toluene

n-Hexyl substituted C4P was prepared as previously reported in the literature.[1] A solution of CsBr in methanol (Sigma-Aldrich) was prepared by dropping a saturated aqueous solution of CsBr into methanol, and mixed with a solution of hexyl-substituted C4P in toluene (Sigma-Aldrich) (mole ratio CsBr:C4P was 1:1.1). The mixture was left over night and then evaporated on a rotary evaporator. The residue was dissolved in toluene to 25 mM CsBr. Collection and analysis of EXAFS data was conducted using the procedure reported previously in our publications.[2] Briefly, the Cs L3-edge and Br K-Edge spectra were collected in fluorescence mode at beamline 12-BM-B at the Advanced Photon Source (APS) at Argonne National Laboratory. A 13-element Ge detector (Canberra) was used to detect the fluorescence signal at a sample-to-detector distance of 1 cm (for Cs) and 40 cm (for Br). The solution was injected into 1 mm Kapton capillaries. Six 1 hr scans were averaged for each solution. Analyses of the k3χ(k) EXAFS was performed using EXAFSPAK. Curve-fitting used theoretical phase and amplitude functions that were calculated with FEFF8.01.

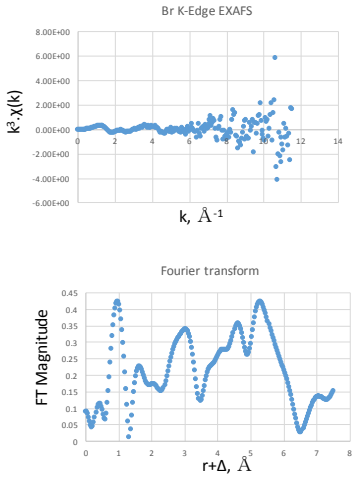

Figure S1. Br K-edge EXAFS and FT-EXAFS for Cs-C4P-Br toluene solution.

ESI1: References

1. N. J. Williams, V. S. Bryanstev, R. Custelcean, C.A. Seipp and B. A. Moyer, *Supramol. Chem.* 2016, **28**, 176-187.
2. R. J. Ellis, Y, Meridiano, R. Chiarizia, L. Berthon, J. Muller, L. Couston and M. R. Antonio, *Chem.-Eur. J.* 2013, **19**, 2663-2675.

ESI2: Computational Details

Electronic structure calculations were carried out using the Gaussian 09[1] Revision D.01 software packages using the M06-2X[2] flavor of density functional. The 6-311+G(d,p) basis set was employed for hydrogen and main group elements. Cs was modeled using the 46MWB effective core potential (ECP46MWB) and the associated basis set,[3] while Br was modeled using ECP28MWB[4] and the VTZ (14s10p2d1f)/[3s3p2d1f]) basis set.[5] The M06-2X density functional was chosen because it provides a relatively accurate prediction of interaction energies in noncovalent complexes.[2,6] Additional calculations were performed with the ωB97X-D function,[7] which is also known to provide accurate binding energies in noncovalent complexes.[6] Using the gas phase geometries, implicit solvent corrections for toluene as a solvent were obtained with the SMD model[8] in Gaussian 09.[1]

All-atom molecular dynamics simulations were performed with the MedeA platform[9] using the MedeA LAMMPS[10] interface module. We employed the non-polarizable PCFF+ forcefield, which is based on the PCFF forcefield[11] with extension to additional molecular classes and refinements, in particular for non-bonded parameters, to reproduce densities and cohesive energies of molecular liquids in a fashion similar to that used in the development of the COMPASS forcefield.[12] The Waldman and Hagler 6th order combination rules were used for the off-diagonal L-J-9-6 parameters. In order to substantially improve the agreement between the computed PCFF+ and experimental crystal structure containing Cs-C4P-Br (LAMVAX ref code), as well as the PCFF+ and M06-2X structures of the Cs-C4P-Br complex in the gas phase, the non-bonded L-J-9-6 ε parameters for Cs and Br were changed from their default values of 0.1475 and 0.07993 kcal/mol to the values of 0.850 and 0.150 kcall/mol, respectively. A full list of forcefield parameters in the LAMMPS format is given at the end of the ESI.

The initial configuration for MD simulations was generated using the MedeA Amorphous Cell Builder[9] by randomly distributing one Cs-C4P^{L}-Br complex and 353 toluene solvent molecules in a periodic cubic box of 40 Å length, which closely corresponds to the experimental density of toluene, $\rho = 0.867$ g/cm^3, at T = 298 K. The dispersion interactions were evaluated using a non-bonded cutoff of 9.5-11 Å with an added long-range Van der Waals tail correction. The long-range electrostatic interaction was calculated by means of the Particle–Particle-Particle–Mesh (P3M) Ewald summation method[13] with long-range precision smaller than 10^{-5} for the electrostatic energy. The initial structure of was first minimized with 1000 steps using the steepest descent method, followed by 2 ns of equilibration at 298 K in a canonical NVT ensemble and another 2 ns of equilibration at 298 K in an NPT ensemble. The average equilibrium volume from the NPT simulations was taken for the subsequent NVT simulations that were performed for 6 ns. The data for the last 5 ns were used for the analyses. The equations of motion were integrated with a time step of 1 fs. The temperature was controlled by the Nosé-Hoover thermostat and barostat with a temperature (Tdamp) and pressure damping (Pdamp) of 100 fs and a friction coefficient (drag) of 1.0 (NVT) and 0 (NPT). Graphical visualization of the complexes and the analyses of the trajectory were performed with VMD.[14]

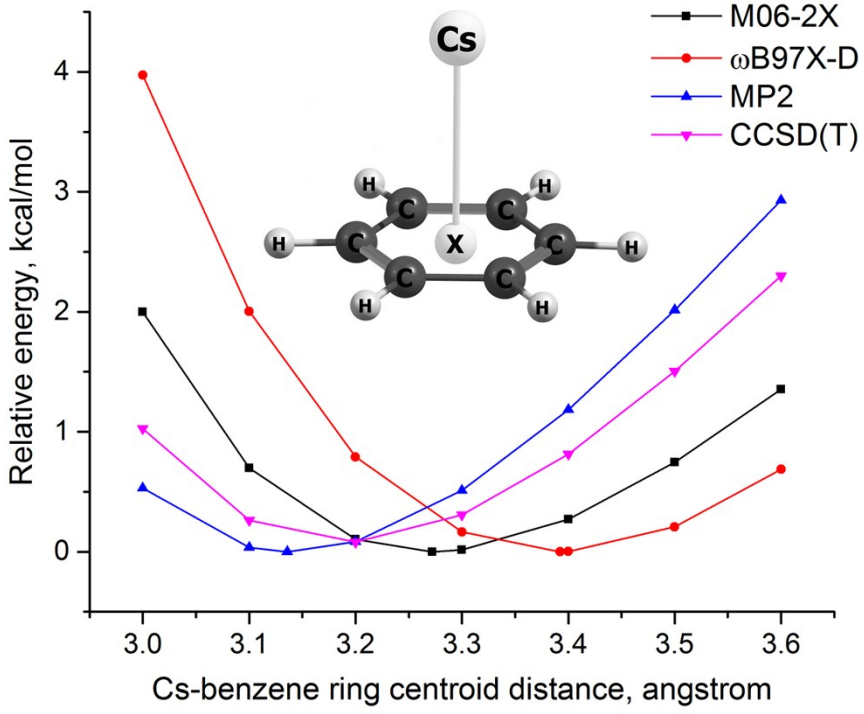

Figure S2. Potential energy surfaces for displacing the Cs^+ cation along the C_6 symmetry axis of benzene. The 6-311+G(d,p)/ECP46MWB(7s6p)/[5s4p](Cs) basis set was employed with M06-2X and ωB97X-D. The aug-cc-pVDZ/ECP46MDF(12s11p5d3f)/[8s8p5d3f](Cs)[15] basis set was employed with MP2 and CCSD(T).

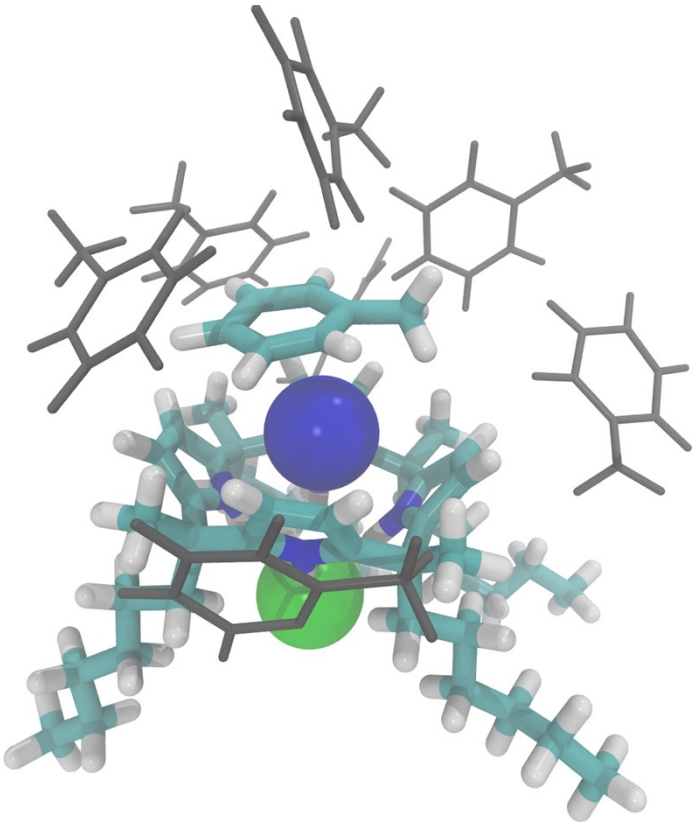

Figure S3. Snapshot of the Cs-C4P^{L}-Br complex in toluene from classical molecular dynamics simulations. Color scheme: Br, green; Cs, magenta; N, blue; H, white; C grey. Solvent molecules with the Cs−C distance in the range of 4−7 Å are shown with thin grey bonds.

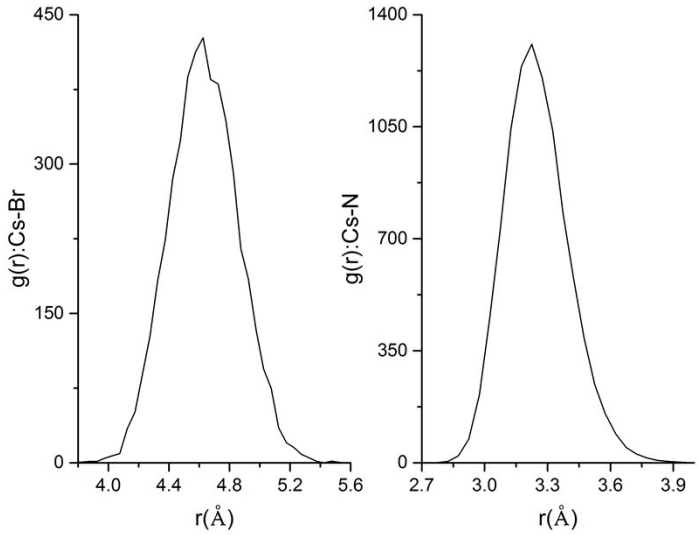

Figure S4. Cs−Br (left) and Cs−N (right) radial distribution functions for the Cs-C4P^{L}-Br complex in toluene obtained from classical molecular dynamics simulations.

Table S1. Comparison of the optimized Cs−C distances in Cs^+-toluene and Cs^+-benzene systems obtained with DFT and post-Hartree-Fock wave function methods[a]

Distance (Å)	M06-2X	ωB97X-D	MP2	CCSD(T)
C(toluene)	3.530	3.603	3.415	
C(toluene)	3.530	3.607	3.415	
C(toluene)	3.533	3.645	3.418	
C(toluene)	3.554	3.665	3.432	
CH_3(toluene)	4.449	4.431	4.349	
C(benzene)	3.557	3.665	3.440	3.489

The 6-311+G(d,p)/ECP46MWB(7s6p)/[5s4p](Cs) basis set was employed with M06-2X and ωB97X-D. The aug-cc-pVDZ/ECP46MDF(12s11p5d3f)/[8s8p5d3f](Cs) basis set was employed with MP2 and CCSD(T).

Table S2. DFT optimized Cs−ligand and Cs−solvent distances in Cs-C4P-Br

Distance (Å)[a]	M06-2X				ωB97X-D
	Cs-C4P^L-Br	Cs-C4P-Br (toluene)	Cs-C4P-Br (toluene)$_2$-B	Cs-C4P-Br (toluene)$_2$-A	Cs-C4P-B$^-$ (toluene)$_2$-A
C_α(pyrrole)	3.678	3.664	3.664	3.551 3.583 3.829 4.250	3.645 3.668 3.902
C_β(pyrrole)	3.466	3.451	3.460	3.473 3.482 3.532 3.766	4.080
C_{meso}	4.122	4.099	4.108	4.131 4.139 4.278 4.287	3.535 3.547 3.612
N	3.304	3.300	3.312	3.321 3.394 3.399 3.422	3.700
Br	4.724	4.597	4.615	4.825	4.210 4.223 4.271
C(toluene)		3.519	3.478 6.296	3.559 3.775	4.272
C(toluene)		3.520	3.500 6.404	3.590 4.061	3.404 3.430 3.444
C(toluene)		3.533	3.541 6.608	3.641 4.781	3.449
C(toluene)		3.543	3.576 6.807	3.678 5.246	4.850
C(toluene)		3.561	3.602 6.807	3.733 5.818	3.600 3.782
C(toluene)		3.565	3.624 7.008	3.747 6.014	3.626 4.086
CH_3(toluene)		4.297	4.354 6.578	4.409 3.665	3.701 4.741
					3.743 5.242
					3.808 5.764
					3.826 5.975
					4.296 3.752

[a]Distances between Cs(I) and ligand atoms are averaged (i) over all pyrrole rings in Cs-C4P-Br(toluene) and Cs-C4P-Br(toluene)$_2$-B and (ii) for each pyrrole ring in Cs-C4P-Br(toluene)$_2$-A. The lipophilic *n*-hexyl substituted C4P is denoted as C4P^L.

Table S3. Comparison of the simulated (DFT) Cs-ligand distances in the Cs-C4P-Br complex in gas phase, solid crystalline (both simulations and experimental[16]) and solution (toluene) phases.

Distance (Å)[a]	Cs-C4P-Br, gas phase			Cs-C4P-Br, solid state			Cs-C4P^L-Br solution
	M06-2X	default pcff+	modified pcff+	default pcff+	modified pcff+	Experimental X-ray[15]	modified pcff+
C_α(pyrrole)	3.654	3.650	3.733	3.813	3.792	3.756	3.789±0.270
C_β(pyrrole)	3.452	3.211	3.414	3.496	3.597	3.595	3.480±0.154
C_{meso}	4.102	3.816	4.045	4.139	4.248	4.245	4.121±0.150
N	3.304	2.930	3.208	3.272	3.466	3.460	3.266±0.155
Br	4.600	3.564	4.424	4.694	5.063	4.946	4.654±0.225
Br (ion pair)				3.265	3.638	3.588	

[a]Distances between Cs(I) and ligand atoms are averaged over all pyrrole rings. The lipophilic *n*-hexyl substituted C4P is denoted as C4P^L.

ESI2: References

1. Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
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Cartesian coordinates and electronic energies of the studied complexes obtained at the M06-2X/6-311+G(d,p)/ ECP46MWB(Cs)/ECP28MWB VTZ(Br) level.

Cs-C4P-Br; E(RM062X) = -1341.08388679 A.U.

Br	19.8941	17.2532	22.7657
N	21.5782	19.6868	21.0133
H	21.2004	18.8252	21.4112
C	21.0503	20.3486	19.9276
N	21.6107	19.6777	24.4992
H	21.2269	18.8168	24.1060
C	21.8079	21.4834	19.7377
H	21.6714	22.2100	18.9526
C	22.8241	21.4974	20.7353
H	23.6010	22.2370	20.8473
C	22.6643	20.3706	21.5116
C	23.4310	19.9159	22.7400
C	22.6869	20.3648	23.9839
C	22.8605	21.4878	24.7625
H	23.6341	22.2288	24.6388
C	21.8629	21.4685	25.7788
H	21.7397	22.1920	26.5689
C	21.1025	20.3343	25.5975
C	19.8819	19.8457	26.3556
C	24.8157	20.5770	22.7288
H	25.3626	20.2731	21.8344
H	25.3783	20.2699	23.6122
C	19.8840	20.4780	27.7536
H	20.7825	20.1754	28.2942
H	19.0050	20.1468	28.3094
C	23.6215	18.3899	22.7346
H	22.6777	17.8410	22.7419
H	24.1752	18.0936	21.8408
C	19.9107	18.3162	26.5146
H	19.0345	17.9909	27.0800
H	19.9094	17.7866	25.5597
N	18.1250	19.6179	24.5314
H	18.5307	18.7707	24.1303
C	18.6302	20.2904	25.6215
N	18.0931	19.6281	21.0456
H	18.5068	18.7794	21.4350
C	17.8360	21.3990	25.8167
H	17.9485	22.1255	26.6057
C	16.8203	21.3851	24.8185
H	16.0191	22.0988	24.7102

C	17.0173	20.2685	24.0362
C	16.2665	19.7943	22.8055
C	16.9937	20.2753	21.5634
C	16.7816	21.3951	20.7896
H	15.9821	22.1076	20.9155
C	17.7795	21.4145	19.7736
H	17.8769	22.1444	18.9858
C	18.5782	20.3061	19.9499
C	19.8154	19.8646	19.1903
C	14.8592	20.4051	22.8204
H	14.3242	20.0773	23.7135
H	14.3076	20.0820	21.9358
C	19.7918	20.5043	17.7958
H	18.9032	20.1754	17.2541
H	20.6807	20.2051	17.2375
C	16.1306	18.2623	22.8026
H	17.0933	17.7469	22.7914
H	15.5885	17.9414	23.6950
C	19.8403	18.3360	19.0229
H	20.7283	18.0441	18.4577
H	19.8580	17.8016	19.9749
H	19.8659	21.5681	27.7074
H	14.8889	21.4959	22.8229
H	19.7741	21.5940	17.8481
H	24.7471	21.6660	22.7315
H	24.1917	18.0893	23.6165
H	20.8099	18.0219	27.0605
H	18.9529	18.0138	18.4733
H	15.5708	17.9464	21.9194
Cs	19.8150	21.8521	22.7812

Cs-C4P-Br(toluene); E(RM062X) = -1612.60616447 A.U.

C	20.7662	25.1495	23.7218
C	21.7133	24.8347	22.7478
C	21.3307	24.7096	21.4169
C	19.9977	24.8876	21.0307
C	19.0597	25.2068	22.0141
C	19.4388	25.3398	23.3497
H	21.0624	25.2423	24.7597
H	22.7485	24.6774	23.0279
H	22.0695	24.4539	20.6647
H	18.0212	25.3483	21.7331
H	18.6946	25.5855	24.0985
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N	21.5753	19.6883	21.0199
H	21.1873	18.8349	21.4260

C	21.0564	20.3454	19.9272
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H	21.2297	18.8135	24.1121
C	21.8311	21.4665	19.7238
H	21.7123	22.1797	18.9232
C	22.8466	21.4780	20.7224
H	23.6355	22.2061	20.8273
C	22.6697	20.3642	21.5121
C	23.4317	19.9133	22.7445
C	22.6864	20.3637	23.9873
C	22.8565	21.4896	24.7631
H	23.6282	22.2324	24.6379
C	21.8603	21.4687	25.7803
H	21.7348	22.1935	26.5689
C	21.1042	20.3308	25.6027
C	19.8842	19.8405	26.3608
C	24.8164	20.5745	22.7357
H	25.3657	20.2706	21.8428
H	25.3769	20.2683	23.6208
C	19.8869	20.4711	27.7595
H	20.7861	20.1685	28.2992
H	19.0084	20.1387	28.3156
C	23.6227	18.3872	22.7416
H	22.6786	17.8388	22.7446
H	24.1803	18.0901	21.8504
C	19.9147	18.3109	26.5179
H	19.0392	17.9839	27.0835
H	19.9130	17.7825	25.5623
N	18.1246	19.6109	24.5398
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C	18.6314	20.2844	25.6283
N	18.0975	19.6280	21.0508
H	18.5169	18.7841	21.4449
C	17.8386	21.3940	25.8228
H	17.9534	22.1219	26.6101
C	16.8231	21.3807	24.8247
H	16.0241	22.0965	24.7148
C	17.0191	20.2636	24.0429
C	16.2696	19.7914	22.8106
C	16.9960	20.2723	21.5677
C	16.7775	21.3880	20.7899
H	15.9742	22.0967	20.9138
C	17.7738	21.4080	19.7728
H	17.8609	22.1313	18.9779
C	18.5797	20.3051	19.9533
C	19.8175	19.8678	19.1917

C	14.8625	20.4029	22.8258
H	14.3273	20.0742	23.7185
H	14.3106	20.0814	21.9406
C	19.7921	20.5153	17.8009
H	18.9023	20.1908	17.2585
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C	16.1327	18.2594	22.8058
H	17.0952	17.7439	22.7932
H	15.5910	17.9377	23.6982
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H	19.8679	21.5611	27.7140
H	14.8934	21.4936	22.8301
H	19.7744	21.6055	17.8593
H	24.7465	21.6637	22.7380
H	24.1887	18.0871	23.6264
H	20.8146	18.0165	27.0626
H	18.9522	18.0207	18.4671
H	15.5723	17.9450	21.9223
Cs	19.8153	21.8435	22.7874
C	19.5995	24.7064	19.5899
H	19.7778	23.6729	19.2797
H	18.5429	24.9293	19.4381
H	20.1876	25.3571	18.9386

Cs-C4P-Br(toluene)$_2$-A; E(RM062X) = -1884.12445097A.U.

Br	19.6891	19.5024	20.1622
N	21.5252	21.9492	18.5935
H	20.9952	21.2011	19.0475
C	21.1821	22.5342	17.3934
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H	21.1307	20.9202	21.5661
C	22.2220	23.3559	17.0275
H	22.2693	23.9599	16.1350
C	23.2245	23.2593	18.0356
H	24.1730	23.7732	18.0441
C	22.7736	22.3773	18.9906
C	23.4333	21.8947	20.2670
C	22.6701	22.3923	21.4807
C	22.9026	23.4821	22.2919
H	23.7227	24.1759	22.1962
C	21.9018	23.4909	23.3051
H	21.8176	24.1959	24.1170
C	21.0822	22.4032	23.0922
C	19.8569	21.9366	23.8563

C	24.8600	22.4547	20.3237
H	25.4328	22.0974	19.4659
H	25.3505	22.1215	21.2397
C	19.9198	22.5077	25.2782
H	20.8186	22.1463	25.7805
H	19.0435	22.1880	25.8451
C	23.5123	20.3563	20.2729
H	22.5304	19.8836	20.1992
H	24.1066	20.0221	19.4196
N	18.1371	21.9482	21.9858
H	18.5398	21.1473	21.4925
C	18.6057	22.4569	23.1772
N	18.1393	22.1215	18.5647
H	18.4425	21.2017	18.8882
C	17.7700	23.4889	23.5357
H	17.8551	24.0847	24.4308
C	16.7646	23.6000	22.5327
H	15.9410	24.2969	22.5235
C	17.0106	22.6338	21.5855
C	16.2860	22.3357	20.2883
C	17.1084	22.8444	19.1189
C	17.0381	24.0382	18.4335
H	16.3197	24.8241	18.6049
C	18.0507	24.0211	17.4312
H	18.2340	24.7834	16.6900
C	18.7163	22.8173	17.5281
C	19.8620	22.2635	16.7019
C	14.9401	23.0708	20.2950
H	14.3339	22.7280	21.1355
H	14.4050	22.8696	19.3654
C	19.8670	22.9675	15.3393
H	18.9172	22.7940	14.8306
H	20.6759	22.5735	14.7213
C	16.0173	20.8264	20.1530
H	16.9318	20.2300	20.1713
H	15.3875	20.4954	20.9817
C	19.6819	20.7517	16.4691
H	20.4881	20.3874	15.8288
H	19.7096	20.1771	17.3970
H	19.9450	23.5989	25.2748
H	15.0705	24.1510	20.3870
H	20.0116	24.0451	15.4423
H	24.8669	23.5468	20.3070
Cs	19.9090	24.3122	20.4679
C	19.4344	28.0111	20.3033
C	18.1659	27.4808	20.0493

C	17.4906	26.8467	21.0937
C	18.0659	26.7441	22.3591
C	19.3374	27.2578	22.5949
C	20.0200	27.8951	21.5597
C	17.5690	27.5892	18.6710
C	21.6029	26.6657	18.0514
C	22.4227	27.1741	19.0613
C	22.6771	28.5476	19.0815
C	22.1182	29.3924	18.1283
C	21.2911	28.8753	17.1334
C	21.0391	27.5078	17.0963
H	21.4295	25.5954	17.9867
H	23.3237	28.9577	19.8513
H	22.3295	30.4550	18.1592
H	20.8580	29.5327	16.3889
H	20.4091	27.0909	16.3180
C	22.9877	26.2717	20.1265
H	24.0128	26.5508	20.3818
H	22.3969	26.3404	21.0483
H	22.9886	25.2285	19.8025
H	19.9620	28.5260	19.5082
H	16.5040	26.4289	20.9176
H	17.5241	26.2528	23.1564
H	19.7855	27.1726	23.5781
H	21.0048	28.3177	21.7293
H	16.4892	27.4337	18.6909
H	17.7721	28.5702	18.2369
H	18.0075	26.8385	18.0068
H	23.9902	20.0122	21.1934
C	19.8228	20.4007	23.9492
H	18.9552	20.0924	24.5370
H	19.7519	19.9175	22.9725
H	20.7286	20.0403	24.4425
H	18.7255	20.5615	15.9759
H	15.4980	20.6251	19.2131

Cs-C4P-Br(toluene)$_2$-B; E(RM062X) = -1884.12107444A.U.

Br	19.9427	29.2862	22.0080
N	18.3885	26.3066	22.7548
H	18.7612	27.2565	22.7216
C	17.1806	25.9154	22.2219
N	21.8113	26.3982	22.1131
H	21.3909	27.3236	22.2178
C	17.0631	24.5601	22.4402
H	16.2200	23.9459	22.1625
C	18.2329	24.1261	23.1265

H	18.4422	23.1223	23.4653
C	19.0375	25.2268	23.3128
C	20.4124	25.3265	23.9457
C	21.4716	25.2935	22.8604
C	22.2180	24.2381	22.3846
H	22.2086	23.2339	22.7785
C	23.0331	24.7275	21.3240
H	23.7576	24.1624	20.7595
C	22.7658	26.0707	21.1766
C	23.3056	27.0675	20.1675
C	20.6124	24.1135	24.8632
H	19.8473	24.1118	25.6424
H	21.5995	24.1594	25.3275
C	24.6376	26.5389	19.6195
H	25.3559	26.4319	20.4343
H	25.0365	27.2376	18.8819
C	20.5355	26.6059	24.7907
H	21.5242	26.6471	25.2534
H	20.4012	27.5174	24.2044
C	23.5585	28.4331	20.8283
H	22.6542	28.8761	21.2502
H	24.2850	28.3195	21.6361
N	21.2071	27.9995	19.0765
H	20.9411	28.5699	19.8809
C	22.3236	27.1971	19.0173
N	17.7754	27.9006	19.7206
H	18.2865	28.4881	20.3821
C	22.2953	26.5534	17.7994
H	23.0414	25.8681	17.4292
C	21.1291	26.9882	17.1072
H	20.8252	26.6921	16.1158
C	20.4719	27.8873	17.9181
C	19.1551	28.6107	17.7060
C	18.0416	27.8233	18.3719
C	17.1783	26.8896	17.8421
H	17.1139	26.6063	16.8034
C	16.3669	26.3986	18.9043
H	15.5727	25.6738	18.8200
C	16.7533	27.0428	20.0593
C	16.2603	26.8700	21.4843
C	18.8719	28.6851	16.1998
H	19.6698	29.2383	15.7012
H	17.9223	29.1948	16.0273
C	14.8517	26.2636	21.4449
H	14.8423	25.2961	20.9402
H	14.1764	26.9334	20.9093

C	19.2212	30.0437	18.2597
H	19.4195	30.0778	19.3329
H	20.0167	30.5953	17.7535
C	16.1869	28.2270	22.2049
H	17.1570	28.7231	22.2777
H	15.5091	28.8924	21.6651
H	24.5200	25.5663	19.1388
H	18.8120	27.6935	15.7487
H	14.4813	26.1222	22.4619
H	20.5299	23.1730	24.3147
Cs	19.6584	25.1848	19.9115
C	16.3062	21.6013	24.6298
C	16.6371	20.8342	23.5101
C	17.9136	20.2737	23.4432
C	18.8359	20.4707	24.4683
C	18.4914	21.2325	25.5798
C	17.2217	21.7986	25.6566
H	15.3219	22.0546	24.6923
H	18.1887	19.6782	22.5781
H	19.8218	20.0245	24.3988
H	19.2084	21.3889	26.3771
H	16.9475	22.4028	26.5134
C	15.6328	20.6198	22.4056
H	16.0730	20.0715	21.5711
H	14.7723	20.0521	22.7680
H	15.2563	21.5742	22.0263
C	19.7676	21.7848	20.6345
C	20.6425	21.8025	19.5465
C	20.1088	22.0113	18.2691
C	18.7420	22.1927	18.0833
C	17.8791	22.1702	19.1785
C	18.3973	21.9655	20.4527
H	20.1576	21.6512	21.6399
H	20.7761	22.0342	17.4133
H	18.3502	22.3556	17.0859
H	16.8148	22.3218	19.0400
H	17.7445	21.9745	21.3162
C	22.1249	21.6022	19.7255
H	22.4294	20.6235	19.3454
H	22.6880	22.3620	19.1785
H	22.4067	21.6639	20.7769
H	19.7782	26.5986	25.5780
H	15.8057	28.0834	23.2185
H	18.2709	30.5509	18.0778
H	23.9608	29.1294	20.0890

Cs-C4P^{L}-Br; E(RM062X) = -2127.16159580 A.U.

Br	-0.0005	-0.9152	-0.0007
N	1.6687	1.5784	-1.8014
H	1.2856	0.7264	-1.3925
C	1.1386	2.2381	-2.8885
N	1.7792	1.5855	1.6548
H	1.3779	0.7198	1.2911
C	1.9298	3.3427	-3.1143
H	1.8002	4.0616	-3.9074
C	2.9710	3.3373	-2.1415
H	3.7761	4.0503	-2.0626
C	2.7928	2.2296	-1.3432
C	3.5760	1.7524	-0.1338
C	2.8725	2.2330	1.1212
C	3.1045	3.3445	1.8990
H	3.9022	4.0566	1.7586
C	2.1303	3.3560	2.9398
H	2.0537	4.0764	3.7387
C	1.3264	2.2518	2.7727
C	0.1315	1.7818	3.5807
C	4.9817	2.3638	-0.1806
H	5.5066	2.0127	-1.0714
H	5.5488	2.0745	0.7051
C	0.1908	2.4274	4.9709
H	1.1193	2.1577	5.4748
H	-0.6549	2.0870	5.5718
C	3.6785	0.2115	-0.1535
H	2.6757	-0.2266	-0.1479
H	4.1245	-0.0757	-1.1111
C	4.4696	-0.4013	1.0080
H	4.2943	0.1809	1.9206
H	5.5442	-0.3468	0.8029
C	4.0653	-1.8564	1.2611
H	4.6565	-2.2620	2.0905
H	3.0156	-1.8778	1.5821
C	4.2249	-2.7681	0.0466
H	5.2638	-2.7296	-0.3071
H	3.5983	-2.4050	-0.7757
C	3.8404	-4.2149	0.3483
H	4.4362	-4.5793	1.1938
H	2.7934	-4.2394	0.6703
C	4.0291	-5.1359	-0.8541
H	3.7470	-6.1646	-0.6210
H	5.0722	-5.1398	-1.1819
H	3.4168	-4.8029	-1.6961
C	0.1357	0.2417	3.7191

H	-0.7414	-0.0447	4.3098
H	-0.0005	-0.2193	2.7359
C	1.4061	-0.3454	4.3358
H	1.4617	-0.1136	5.4047
H	2.2852	0.1174	3.8706
C	1.4856	-1.8573	4.1316
H	0.6592	-2.3506	4.6574
H	1.3412	-2.0766	3.0664
C	2.8170	-2.4472	4.5888
H	2.9199	-2.3410	5.6757
H	3.6341	-1.8648	4.1452
C	2.9823	-3.9129	4.1959
H	2.1950	-4.5079	4.6714
H	2.8299	-4.0070	3.1153
C	4.3532	-4.4718	4.5670
H	4.4511	-5.5210	4.2800
H	4.5283	-4.4000	5.6439
H	5.1478	-3.9122	4.0646
N	-1.6687	1.5796	1.7993
H	-1.2859	0.7273	1.3906
C	-1.1383	2.2393	2.8862
N	-1.7792	1.5858	-1.6569
H	-1.3782	0.7201	-1.2930
C	-1.9291	3.3443	3.1117
H	-1.7992	4.0633	3.9047
C	-2.9703	3.3390	2.1389
H	-3.7751	4.0523	2.0599
C	-2.7925	2.2310	1.3409
C	-3.5760	1.7539	0.1316
C	-2.8722	2.2339	-1.1235
C	-3.1039	3.3452	-1.9016
H	-3.9013	4.0576	-1.7613
C	-2.1297	3.3561	-2.9424
H	-2.0527	4.0762	-3.7415
C	-1.3261	2.2516	-2.7750
C	-0.1314	1.7809	-3.5829
C	-4.9814	2.3659	0.1782
H	-5.5064	2.0152	1.0691
H	-5.5486	2.0765	-0.7074
C	-0.1905	2.4262	-4.9733
H	-1.1191	2.1567	-5.4771
H	0.6550	2.0852	-5.5740
C	-3.6791	0.2130	0.1518
H	-2.6764	-0.2256	0.1464
H	-4.1252	-0.0737	1.1095
C	-4.4704	-0.3998	-1.0095

H -4.2948 0.1819 -1.9223
H -5.5450 -0.3448 -0.8045
C -4.0668 -1.8552 -1.2621
H -4.6582 -2.2608 -2.0913
H -3.0171 -1.8772 -1.5832
C -4.2267 -2.7663 -0.0472
H -5.2656 -2.7272 0.3065
H -3.5999 -2.4032 0.7749
C -3.8429 -4.2134 -0.3483
H -4.4389 -4.5780 -1.1936
H -2.7959 -4.2385 -0.6705
C -4.0318 -5.1338 0.8545
H -3.7502 -6.1627 0.6219
H -5.0749 -5.1370 1.1825
H -3.4192 -4.8006 1.6963
C -0.1362 0.2408 -3.7208
H 0.7407 -0.0461 -4.3115
H -0.0001 -0.2200 -2.7375
C -1.4070 -0.3460 -4.3371
H -1.4626 -0.1144 -5.4061
H -2.2859 0.1172 -3.8719
C -1.4871 -1.8578 -4.1326
H -0.6609 -2.3515 -4.6584
H -1.3427 -2.0769 -3.0673
C -2.8187 -2.4473 -4.5896
H -2.9216 -2.3414 -5.6765
H -3.6356 -1.8643 -4.1462
C -2.9847 -3.9127 -4.1962
H -2.1977 -4.5083 -4.6715
H -2.8324 -4.0065 -3.1155
C -4.3558 -4.4712 -4.5671
H -4.4542 -5.5202 -4.2798
H -4.5309 -4.3996 -5.6440
H -5.1502 -3.9110 -4.0649
H 0.1478 3.5161 4.9091
H -4.9439 3.4559 0.2115
H -0.1469 3.5149 -4.9118
H 4.9446 3.4539 -0.2141
Cs 0.0004 3.8085 -0.0013

LAMMPS parameters.dat file

```
bond_coeff          1 1.53 299.67 -501.77 679.81   # c     c
bond_coeff          2 1.101 345 -691.89 844.6      # c     h
bond_coeff          3 1.53 299.67 -501.77 679.81   # c     c
bond_coeff          4 1.0982 372.83 -803.45 894.32 # cp    h
bond_coeff          5 1.417 470.84 -627.62 1327.6  # cp    cp
bond_coeff          6 1.53 299.67 -501.77 679.81   # c     c
bond_coeff          7 1.101 345 -691.89 844.6      # c     h
```

```
bond_coeff          8 1.501 321.9 -521.82 572.16   # c     cp
bond_coeff          9 1.53 299.67 -501.77 679.81   # c     c
bond_coeff         10 1.0012 465.86 -1066.2 1496.6 # h*    nn
bond_coeff         11 1.3912 447.04 -784.53 886.17 # cp    nn
bond_coeff         12 1.501 321.9 -521.82 572.16   # c     cp
angle_coeff         1 111.87 40.837 -15.667 0      # cp    nn      h*
angle_coeff         2 120 50 0 0   # *     n       *
angle_coeff         3 121.46 61.065 -21.617 0      # cp    cp      nn
angle_coeff         4 120.05 44.715 -22.735 0      # c     cp      cp
angle_coeff         5 120 65 0 0   # *     cp      *
angle_coeff         6 117.94 35.156 -12.468 0      # cp    cp      h
angle_coeff         7 118.9 61.023 -34.993 0       # cp    cp      cp
angle_coeff         8 112.67 39.516 -7.443 -9.5583 # c     c       c
angle_coeff         9 108.4 43.959 -8.3924 -9.3379 # c     c       cp
angle_coeff        10 108.4 43.959 -8.3924 -9.3379 # c     c       cp
angle_coeff        11 111 44.323 -9.4454 0 # cp    c       cp
angle_coeff        12 110.77 41.453 -10.604 5.129  # c     c       h
angle_coeff        13 107.66 39.641 -12.921 -2.4318       # h     c       h
angle_coeff        14 110.77 41.453 -10.604 5.129  # c     c       h
angle_coeff        15 110.77 41.453 -10.604 5.129  # c     c       h
angle_coeff        16 107.66 39.641 -12.921 -2.4318       # h     c       h
angle_coeff        17 112.67 39.516 -7.443 -9.5583 # c     c       c
angle_coeff        18 112.67 39.516 -7.443 -9.5583 # c     c       c
angle_coeff        19 110.77 41.453 -10.604 5.129  # c     c       h
angle_coeff        20 112.67 39.516 -7.443 -9.5583 # c     c       c
angle_coeff        21 110.77 41.453 -10.604 5.129  # c     c       h
angle_coeff        22 120.05 44.715 -22.735 0      # c     cp      cp
angle_coeff        23 111 44.323 -9.4454 0 # cp    c       h
dihedral_coeff      1 0 0 1.219 0 0 0      # cp    cp      nn      h*
dihedral_coeff      2 0 0 2.25 0 0 0       # *     cp      n       *
dihedral_coeff      3 0 0 2.25 0 0 0       # *     cp_     n_      *
dihedral_coeff      4 0 0 2.25 0 0 0       # *     cp_     n_      *
dihedral_coeff      5 0 0 1.3331 0 0 0     # h     cp      cp      nn
dihedral_coeff      6 0 0 5.3826 0 0 0     # cp    cp      cp      nn
dihedral_coeff      7 0 0 1.559 0 0 0      # c     cp      cp      h
dihedral_coeff      8 0 0 4.4072 0 0 0     # c     cp      cp      cp
dihedral_coeff      9 -0.2802 0 -0.0678 0 -0.0122 0        # c     c       cp      cp
dihedral_coeff     10 -0.2802 0 -0.0678 0 -0.0122 0        # c     c       cp      cp
dihedral_coeff     11 -0.2802 0 -0.0678 0 -0.0122 0        # cp    c       cp      cp
dihedral_coeff     12 8.3667 0 1.1932 0 0 0        # cp    cp      cp      cp
dihedral_coeff     13 0 0 3.9661 0 0 0     # cp    cp      cp      h
dihedral_coeff     14 0 0 1.8769 0 0 0     # h     cp      cp      h
dihedral_coeff     15 0 0 0.0316 0 -0.1681 0       # c     c       c       h
dihedral_coeff     16 -0.0228 0 0.028 0 -0.1863 0  # cp    c       c       h
dihedral_coeff     17 0 0 0.0316 0 -0.1681 0       # c     c       c       h
dihedral_coeff     18 0 0 0.0514 0 -0.143 0        # c     c       c       c
dihedral_coeff     19 -0.0228 0 0.028 0 -0.1863 0  # cp    c       c       h
dihedral_coeff     20 0 0 0 0 0.158 0      # *     c_      c_      *
dihedral_coeff     21 0 0 0.0316 0 -0.1681 0       # c     c       c       h
dihedral_coeff     22 -0.1432 0 0.0617 0 -0.1083 0 # h     c       c       h
dihedral_coeff     23 0 0 0.0514 0 -0.143 0        # c     c       c       c
dihedral_coeff     24 0 0 0.0316 0 -0.1681 0       # c     c       c       h
dihedral_coeff     25 0 0 0.0514 0 -0.143 0        # c     c       c       c
dihedral_coeff     26 0 0 0.0316 0 -0.1681 0       # c     c       c       h
dihedral_coeff     27 0 0 0.0514 0 -0.143 0        # c     c       c       c
dihedral_coeff     28 -0.1432 0 0.0617 0 -0.1083 0 # h     c       c       h
dihedral_coeff     29 0 0 0.0316 0 -0.1681 0       # c     c       c       h
dihedral_coeff     30 0 0 4.4072 0 0 0     # c     cp      cp      cp
dihedral_coeff     31 0 0 1.559 0 0 0      # c     cp      cp      h
dihedral_coeff     32 -0.2801 0 -0.0678 0 -0.0122 0        # h     c       cp      cp
improper_coeff      1 0.1 0       # *     n       *       *
improper_coeff      2 10 0 # *     cp      *       *
improper_coeff      3 4.8912 0    # cp    cp      cp      h
improper_coeff      4 0.0 0.0     # c2    c0      c3      cp
improper_coeff      5 0.0 0.0     # c3    c0      cp      cp
improper_coeff      6 0.0 0.0     # c2    c0      cp      cp
```

```
improper_coeff      7 0.0 0.0     # c0   c3     hc     hc
improper_coeff      8 0.0 0.0     # hc   c3     hc     hc
improper_coeff      9 0.0 0.0     # c0   c2     c2     hc
improper_coeff     10 0.0 0.0     # c0   c2     hc     hc
improper_coeff     11 0.0 0.0     # c2   c2     hc     hc
improper_coeff     12 0.0 0.0     # c2   c2     c2     hc
improper_coeff     13 0.0 0.0     # c2   c2     c3     hc
improper_coeff     14 0.0 0.0     # c3   c2     hc     hc
improper_coeff     15 0.0 0.0     # c2   c3     hc     hc
improper_coeff     16 7.8153 0    # c    cp     cp     cp
improper_coeff     17 0.0 0.0     # cp   c3     hc     hc
angle_coeff         1 bb 4.5393 1.3912 1.0012     # cp   nn     h*
angle_coeff         2 bb 0.0 1.3912 1.3912 # *     n_     *
angle_coeff         3 bb 46.951 1.417 1.3912      # cp   cp     nn
angle_coeff         4 bb 12.068 1.501 1.417       # c    cp     cp
angle_coeff         5 bb 0.0 1.501 1.3912  # *     cp_    *
angle_coeff         6 bb 1.0795 1.417 1.0982      # cp   cp     h
angle_coeff         7 bb 68.286 1.417 1.417       # cp   cp     cp
angle_coeff         8 bb 0 1.53 1.53       # c    c      c
angle_coeff         9 bb 0 1.53 1.501      # c    c      cp
angle_coeff        10 bb 0 1.53 1.501      # c    c      cp
angle_coeff        11 bb 0.0 1.501 1.501   # cp   c      cp
angle_coeff        12 bb 3.3872 1.53 1.101 # c    c      h
angle_coeff        13 bb 5.3316 1.101 1.101       # h    c      h
angle_coeff        14 bb 3.3872 1.53 1.101 # c    c      h
angle_coeff        15 bb 3.3872 1.53 1.101 # c    c      h
angle_coeff        16 bb 5.3316 1.101 1.101       # h    c      h
angle_coeff        17 bb 0 1.53 1.53      # c    c      c
angle_coeff        18 bb 0 1.53 1.53      # c    c      c
angle_coeff        19 bb 3.3872 1.53 1.101 # c    c      h
angle_coeff        20 bb 0 1.53 1.53      # c    c      c
angle_coeff        21 bb 3.3872 1.53 1.101 # c    c      h
angle_coeff        22 bb 12.068 1.501 1.417       # c    cp     cp
angle_coeff        23 bb 2.9168 1.501 1.101       # cp   c      h
angle_coeff         1 ba 38.57 16.552 1.3912 1.0012      # cp   nn     h*
angle_coeff         2 ba 0.0 0.0 1.3912 1.3912    # *    n_     *
angle_coeff         3 ba 39.404 73.655 1.417 1.3912      # cp   cp     nn
angle_coeff         4 ba 47.058 31.077 1.501 1.417 # c    cp     cp
angle_coeff         5 ba 0.0 0.0 1.501 1.3912     # *    cp     *
angle_coeff         6 ba 20.003 24.218 1.417 1.0982      # cp   cp     h
angle_coeff         7 ba 28.871 28.871 1.417 1.417 # cp   cp     cp
angle_coeff         8 ba 8.016 8.016 1.53 1.53    # c    c      c
angle_coeff         9 ba 0 0 1.53 1.501   # c    c      cp
angle_coeff        10 ba 0 0 1.53 1.501   # c    c      cp
angle_coeff        11 ba 0.0 0.0 1.501 1.501     # cp   c      cp
angle_coeff        12 ba 20.754 11.421 1.53 1.101  # c    c      h
angle_coeff        13 ba 18.103 18.103 1.101 1.101 # h    c      h
angle_coeff        14 ba 20.754 11.421 1.53 1.101  # c    c      h
angle_coeff        15 ba 20.754 11.421 1.53 1.101  # c    c      h
angle_coeff        16 ba 18.103 18.103 1.101 1.101 # h    c      h
angle_coeff        17 ba 8.016 8.016 1.53 1.53    # c    c      c
angle_coeff        18 ba 8.016 8.016 1.53 1.53    # c    c      c
angle_coeff        19 ba 20.754 11.421 1.53 1.101  # c    c      h
angle_coeff        20 ba 8.016 8.016 1.53 1.53    # c    c      c
angle_coeff        21 ba 20.754 11.421 1.53 1.101  # c    c      h
angle_coeff        22 ba 47.058 31.077 1.501 1.417 # c    cp     cp
angle_coeff        23 ba 26.461 11.772 1.501 1.101 # cp   c      h
dihedral_coeff      1 mbt 0 3.2085 0 1.3912       # cp   cp     nn     h*
dihedral_coeff      2 mbt 0.0 0.0 0.0 1.3912      # *    cp     n      *
dihedral_coeff      3 mbt 0.0 0.0 0.0 1.3912      # *    cp     n      *
dihedral_coeff      4 mbt 0.0 0.0 0.0 1.3912      # *    cp     n      *
dihedral_coeff      5 mbt 0 2.2883 0 1.417 # h    cp     cp     nn
dihedral_coeff      6 mbt 0 -0.5693 0 1.417       # cp   cp     cp     nn
dihedral_coeff      7 mbt 0 3.9421 0 1.417 # c    cp     cp     h
dihedral_coeff      8 mbt 0 9.1792 0 1.417 # c    cp     cp     cp
dihedral_coeff      9 mbt 0 0 0 1.501      # c    c      cp     cp
```

```
dihedral_coeff 10 mbt 0 0 0 1.501 # c c cp cp
dihedral_coeff 11 mbt 0.0 0.0 0.0 1.501 # cp c cp cp
dihedral_coeff 12 mbt 27.599 -2.312 0 1.417 # cp cp cp cp
dihedral_coeff 13 mbt 0 -1.1521 0 1.417 # cp cp cp h
dihedral_coeff 14 mbt 0 4.8228 0 1.417 # h cp cp h
dihedral_coeff 15 mbt -14.879 -3.6581 -0.3138 1.53 # c c c h
dihedral_coeff 16 mbt 0 0 0 1.53 # cp c c h
dihedral_coeff 17 mbt -14.879 -3.6581 -0.3138 1.53 # c c c h
dihedral_coeff 18 mbt -17.787 -7.1877 0 1.53 # c c c c
dihedral_coeff 19 mbt 0 0 0 1.53 # cp c c h
dihedral_coeff 20 mbt 0.0 0.0 0.0 1.53 # * c c *
dihedral_coeff 21 mbt -14.879 -3.6581 -0.3138 1.53 # c c c h
dihedral_coeff 22 mbt -14.261 -0.5322 -0.4864 1.53 # h c c h
dihedral_coeff 23 mbt -17.787 -7.1877 0 1.53 # c c c c
dihedral_coeff 24 mbt -14.879 -3.6581 -0.3138 1.53 # c c c h
dihedral_coeff 25 mbt -17.787 -7.1877 0 1.53 # c c c c
dihedral_coeff 26 mbt -14.879 -3.6581 -0.3138 1.53 # c c c h
dihedral_coeff 27 mbt -17.787 -7.1877 0 1.53 # c c c c
dihedral_coeff 28 mbt -14.261 -0.5322 -0.4864 1.53 # h c c h
dihedral_coeff 29 mbt -14.879 -3.6581 -0.3138 1.53 # c c c h
dihedral_coeff 30 mbt 0 9.1792 0 1.417 # c cp cp cp
dihedral_coeff 31 mbt 0 3.9421 0 1.417 # c cp cp h
dihedral_coeff 32 mbt -5.5679 1.4083 0.301 1.501 # h c cp cp
dihedral_coeff 1 ebt 0 -3.7281 0 0 0.2849 0 1.417 1.0012 # cp cp nn h*
dihedral_coeff 2 ebt 0.0 0.0 0.0 0.0 0.0 0.0 1.501 1.0012 # * cp n *
dihedral_coeff 3 ebt 0.0 0.0 0.0 0.0 0.0 0.0 1.417 1.3912 # * cp n *
dihedral_coeff 4 ebt 0.0 0.0 0.0 0.0 0.0 0.0 1.501 1.3912 # * cp n *
dihedral_coeff 5 ebt 0 -2.6482 0 0 -1.6402 0 1.0982 1.3912 # h cp cp nn
dihedral_coeff 6 ebt 0 -6.5404 0 0 -7.3477 0 1.417 1.3912 # cp cp cp nn
dihedral_coeff 7 ebt 0 -1.797 0 0 -0.4879 0 1.501 1.0982 # c cp cp h
dihedral_coeff 8 ebt 0 0.2421 0 0 -0.6918 0 1.501 1.417 # c cp cp cp
dihedral_coeff 9 ebt 0 0 0 0 0 0 1.53 1.417 # c c cp cp
dihedral_coeff 10 ebt 0 0 0 0 0 0 1.53 1.417 # c c cp cp
dihedral_coeff 11 ebt 0.0 0.0 0.0 0.0 0.0 0.0 1.501 1.417 # cp c cp cp
dihedral_coeff 12 ebt -0.1185 6.3204 0 -0.1185 6.3204 0 1.417 1.417 # cp cp cp cp
dihedral_coeff 13 ebt 0 -6.8958 0 0 -0.4669 0 1.417 1.0982 # cp cp cp h
dihedral_coeff 14 ebt 0 -0.689 0 0 -0.689 0 1.0982 1.0982 # h cp cp h
dihedral_coeff 15 ebt 0.2486 0.2422 -0.0925 0.0814 0.0591 0.2219 1.53 1.101 # c c c h
dihedral_coeff 16 ebt 0 0 0 0 0 0 1.501 1.101 # cp c c h
dihedral_coeff 17 ebt 0.2486 0.2422 -0.0925 0.0814 0.0591 0.2219 1.53 1.101 # c c c h
dihedral_coeff 18 ebt -0.0732 0 0 -0.0732 0 0 1.53 1.53 # c c c c
dihedral_coeff 19 ebt 0 0 0 0 0 0 1.501 1.101 # cp c c h
dihedral_coeff 20 ebt 0.0 0.0 0.0 0.0 0.0 0.0 1.501 1.53 # * c c *
dihedral_coeff 21 ebt 0.2486 0.2422 -0.0925 0.0814 0.0591 0.2219 1.53 1.101 # c c c h
dihedral_coeff 22 ebt 0.213 0.312 0.0777 0.213 0.312 0.0777 1.101 1.101 # h c c h
dihedral_coeff 23 ebt -0.0732 0 0 -0.0732 0 0 1.53 1.53 # c c c c
dihedral_coeff 24 ebt 0.2486 0.2422 -0.0925 0.0814 0.0591 0.2219 1.53 1.101 # c c c h
dihedral_coeff 25 ebt -0.0732 0 0 -0.0732 0 0 1.53 1.53 # c c c c
dihedral_coeff 26 ebt 0.2486 0.2422 -0.0925 0.0814 0.0591 0.2219 1.53 1.101 # c c c h
dihedral_coeff 27 ebt -0.0732 0 0 -0.0732 0 0 1.53 1.53 # c c c c
dihedral_coeff 28 ebt 0.213 0.312 0.0777 0.213 0.312 0.0777 1.101 1.101 # h c c h
dihedral_coeff 29 ebt 0.2486 0.2422 -0.0925 0.0814 0.0591 0.2219 1.53 1.101 # c c c h
dihedral_coeff 30 ebt 0 0.2421 0 0 -0.6918 0 1.501 1.417 # c cp cp cp
dihedral_coeff 31 ebt 0 -1.797 0 0 -0.4879 0 1.501 1.0982 # c cp cp h
dihedral_coeff 32 ebt 1.3997 0.7756 0 -0.5835 1.122 0.3978 1.101 1.417 # h c cp cp
dihedral_coeff 1 at 0 1.2616 0 0 0.7744 0 121.46 111.87 # cp cp nn h*
dihedral_coeff 2 at 0.0 0.0 0.0 0.0 0.0 0.0 120 111.87 # * cp n *
dihedral_coeff 3 at 0.0 0.0 0.0 0.0 0.0 0.0 121.46 120 # * cp n *
dihedral_coeff 4 at 0.0 0.0 0.0 0.0 0.0 0.0 120 120 # * cp n *
dihedral_coeff 5 at 0 2.9813 0 0 0.2787 0 117.94 121.46 # h cp cp nn
dihedral_coeff 6 at 0 9.0901 0 0 -6.0882 0 118.9 121.46 # cp cp cp nn
dihedral_coeff 7 at 0 -0.1242 0 0 3.4601 0 120.05 117.94 # c cp cp h
dihedral_coeff 8 at 0 -4.4683 0 0 3.8987 0 120.05 118.9 # c cp cp cp
dihedral_coeff 9 at 0 0 0 0 0 0 108.4 120.05 # c c cp cp
dihedral_coeff 10 at 0 0 0 0 0 0 108.4 120.05 # c c cp cp
dihedral_coeff 11 at 0.0 0.0 0.0 0.0 0.0 0.0 111 120.05 # cp c cp cp
```

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dihedral_coeff      12 at 1.9767 1.0239 0 1.9767 1.0239 0 118.9 118.9      # cp   cp     cp     cp
dihedral_coeff      13 at 0 2.5014 0 0 2.7147 0 118.9 117.94      # cp   cp     cp     h
dihedral_coeff      14 at 0 2.4501 0 0 2.4501 0 117.94 117.94      # h    cp     cp     h
dihedral_coeff      15 at -0.2454 0 -0.1136 0.3113 0.4516 -0.1988 112.67 110.77    # c    c      c      h
dihedral_coeff      16 at 0 0 0 0 0 0 108.4 110.77  # cp   c      c      h
dihedral_coeff      17 at -0.2454 0 -0.1136 0.3113 0.4516 -0.1988 112.67 110.77    # c    c      c      h
dihedral_coeff      18 at 0.3886 -0.3139 0.1389 0.3886 -0.3139 0.1389 112.67 112.67 # c    c      c      c
dihedral_coeff      19 at 0 0 0 0 0 0 108.4 110.77  # cp   c      c      h
dihedral_coeff      20 at 0.0 0.0 0.0 0.0 0.0 0.0 108.4 112.67     # *    c      c      *
dihedral_coeff      21 at -0.2454 0 -0.1136 0.3113 0.4516 -0.1988 112.67 110.77    # c    c      c      h
dihedral_coeff      22 at -0.8085 0.5569 -0.2466 -0.8085 0.5569 -0.2466 110.77 110.77      # h    c      c      h
dihedral_coeff      23 at 0.3886 -0.3139 0.1389 0.3886 -0.3139 0.1389 112.67 112.67 # c    c      c      c
dihedral_coeff      24 at -0.2454 0 -0.1136 0.3113 0.4516 -0.1988 112.67 110.77    # c    c      c      h
dihedral_coeff      25 at 0.3886 -0.3139 0.1389 0.3886 -0.3139 0.1389 112.67 112.67 # c    c      c      c
dihedral_coeff      26 at -0.2454 0 -0.1136 0.3113 0.4516 -0.1988 112.67 110.77    # c    c      c      h
dihedral_coeff      27 at 0.3886 -0.3139 0.1389 0.3886 -0.3139 0.1389 112.67 112.67 # c    c      c      c
dihedral_coeff      28 at -0.8085 0.5569 -0.2466 -0.8085 0.5569 -0.2466 110.77 110.77      # h    c      c      h
dihedral_coeff      29 at -0.2454 0 -0.1136 0.3113 0.4516 -0.1988 112.67 110.77    # c    c      c      h
dihedral_coeff      30 at 0 -4.4683 0 0 3.8987 0 120.05 118.9      # c    cp     cp     cp
dihedral_coeff      31 at 0 -0.1242 0 0 3.4601 0 120.05 117.94     # c    cp     cp     h
dihedral_coeff      32 at 4.6266 0.1632 0.0461 0.2251 0.6548 0.1237 111 120.05     # h    c      cp     cp
dihedral_coeff       1 aat -7.1755 121.46 111.87    # cp   cp     nn     h*
dihedral_coeff       2 aat 0.0 120 111.87   # *    cp     n      *
dihedral_coeff       3 aat 0.0 121.46 120   # *    cp     n      *
dihedral_coeff       4 aat 0.0 120 120      # *    cp     n      *
dihedral_coeff       5 aat 0 117.94 121.46  # h    cp     cp     nn
dihedral_coeff       6 aat 0 118.9 121.46   # cp   cp     cp     nn
dihedral_coeff       7 aat 4.4444 120.05 117.94     # c    cp     cp     h
dihedral_coeff       8 aat -14.41 120.05 118.9      # c    cp     cp     cp
dihedral_coeff       9 aat 0 108.4 120.05   # c    c      cp     cp
dihedral_coeff       10 aat 0 108.4 120.05   # c    c      cp     cp
dihedral_coeff       11 aat 0.0 111 120.05   # cp   c      cp     cp
dihedral_coeff       12 aat 0 118.9 118.9    # cp   cp     cp     cp
dihedral_coeff       13 aat -4.8141 118.9 117.94     # cp   cp     cp     h
dihedral_coeff       14 aat 0.3598 117.94 117.94     # h    cp     cp     h
dihedral_coeff       15 aat -16.164 112.67 110.77    # c    c      c      h
dihedral_coeff       16 aat 0 108.4 110.77   # cp   c      c      h
dihedral_coeff       17 aat -16.164 112.67 110.77    # c    c      c      h
dihedral_coeff       18 aat -22.045 112.67 112.67    # c    c      c      c
dihedral_coeff       19 aat 0 108.4 110.77   # cp   c      c      h
dihedral_coeff       20 aat 0.0 108.4 112.67 # *    c      c      *
dihedral_coeff       21 aat -16.164 112.67 110.77    # c    c      c      h
dihedral_coeff       22 aat -12.564 110.77 110.77    # h    c      c      h
dihedral_coeff       23 aat -22.045 112.67 112.67    # c    c      c      c
dihedral_coeff       24 aat -16.164 112.67 110.77    # c    c      c      h
dihedral_coeff       25 aat -22.045 112.67 112.67    # c    c      c      c
dihedral_coeff       26 aat -16.164 112.67 110.77    # c    c      c      h
dihedral_coeff       27 aat -22.045 112.67 112.67    # c    c      c      c
dihedral_coeff       28 aat -12.564 110.77 110.77    # h    c      c      h
dihedral_coeff       29 aat -16.164 112.67 110.77    # c    c      c      h
dihedral_coeff       30 aat -14.41 120.05 118.9      # c    cp     cp     cp
dihedral_coeff       31 aat 4.4444 120.05 117.94     # c    cp     cp     h
dihedral_coeff       32 aat -5.8888 111 120.05       # h    c      cp     cp
dihedral_coeff       1 bb13 4.2366 1.417 1.0012     # cp   cp     nn     h*
dihedral_coeff       2 bb13 0.0 1.501 1.0012        # *    cp     n      *
dihedral_coeff       3 bb13 0.0 1.417 1.3912        # *    cp     n      *
dihedral_coeff       4 bb13 0.0 1.501 1.3912        # *    cp     n      *
dihedral_coeff       5 bb13 -1.0746 1.0982 1.3912   # h    cp     cp     nn
dihedral_coeff       6 bb13 -9.7999 1.417 1.3912    # cp   cp     cp     nn
dihedral_coeff       7 bb13 0.8743 1.501 1.0982     # c    cp     cp     h
dihedral_coeff       8 bb13 2.5085 1.501 1.417      # c    cp     cp     cp
dihedral_coeff       9 bb13 0.0 1.53 1.417  # c    c      cp     cp
dihedral_coeff       10 bb13 0.0 1.53 1.417  # c    c      cp     cp
dihedral_coeff       11 bb13 0.0 1.501 1.417 # cp   c      cp     cp
dihedral_coeff       12 bb13 53 1.417 1.417  # cp   cp     cp     cp
dihedral_coeff       13 bb13 -6.2741 1.417 1.0982    # cp   cp     cp     h
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dihedral_coeff      14 bb13 -1.7077 1.0982 1.0982   # h    cp     cp     h
dihedral_coeff      15 bb13 0.0 1.53 1.101  # c    c      c      h
dihedral_coeff      16 bb13 0.0 1.501 1.101 # cp   c      c      h
dihedral_coeff      17 bb13 0.0 1.53 1.101  # c    c      c      h
dihedral_coeff      18 bb13 0.0 1.53 1.53   # c    c      c      c
dihedral_coeff      19 bb13 0.0 1.501 1.101 # cp   c      c      h
dihedral_coeff      20 bb13 0.0 1.501 1.53  # *    c      c      *
dihedral_coeff      21 bb13 0.0 1.53 1.101  # c    c      c      h
dihedral_coeff      22 bb13 0.0 1.101 1.101 # h    c      c      h
dihedral_coeff      23 bb13 0.0 1.53 1.53   # c    c      c      c
dihedral_coeff      24 bb13 0.0 1.53 1.101  # c    c      c      h
dihedral_coeff      25 bb13 0.0 1.53 1.53   # c    c      c      c
dihedral_coeff      26 bb13 0.0 1.53 1.101  # c    c      c      h
dihedral_coeff      27 bb13 0.0 1.53 1.53   # c    c      c      c
dihedral_coeff      28 bb13 0.0 1.101 1.101 # h    c      c      h
dihedral_coeff      29 bb13 0.0 1.53 1.101  # c    c      c      h
dihedral_coeff      30 bb13 2.5085 1.501 1.417    # c    cp     cp     cp
dihedral_coeff      31 bb13 0.8743 1.501 1.0982   # c    cp     cp     h
dihedral_coeff      32 bb13 -3.4826 1.101 1.417   # h    c      cp     cp
improper_coeff       1 aa 0.0 0.0 0.0 120.0 120.0 120.0   # *    n_     *      *
improper_coeff       2 aa 0.0 0.0 0.0 120.0 120.0 120.0   # *    cp_    *      *
improper_coeff       3 aa 0 0 0 118.9 117.94 117.94 # cp   cp     cp     h
improper_coeff       4 aa 0.0 0.0 0.0 120.0 120.0 120.0   # c2   c0     c3     cp
improper_coeff       5 aa 0.0 0.0 0.0 120.0 120.0 120.0   # c3   c0     cp     cp
improper_coeff       6 aa 0.0 0.0 0.0 120.0 120.0 120.0   # c2   c0     cp     cp
improper_coeff       7 aa 0.2738 -0.4825 0.2738 110.77 110.77 107.66      # c    c      h      h
improper_coeff       8 aa -0.3157 -0.3157 -0.3157 107.66 107.66 107.66    # h    c      h      h
improper_coeff       9 aa -1.3199 -1.3199 0.1184 112.67 110.77 110.77     # c    c      c      h
improper_coeff      10 aa 0.2738 -0.4825 0.2738 110.77 110.77 107.66      # c    c      h      h
improper_coeff      11 aa 0.2738 -0.4825 0.2738 110.77 110.77 107.66      # c    c      h      h
improper_coeff      12 aa -1.3199 -1.3199 0.1184 112.67 110.77 110.77     # c    c      c      h
improper_coeff      13 aa -1.3199 -1.3199 0.1184 112.67 110.77 110.77     # c    c      c      h
improper_coeff      14 aa 0.2738 -0.4825 0.2738 110.77 110.77 107.66      # c    c      h      h
improper_coeff      15 aa 0.2738 -0.4825 0.2738 110.77 110.77 107.66      # c    c      h      h
improper_coeff      16 aa 0 0 0 120.05 120.05 118.9 # c    cp     cp     cp
improper_coeff      17 aa 2.3794 3.0118 2.3794 111 111 107.66     # cp   c      h      h
pair_coeff              1    1 0.15 5.4135 # Br -
pair_coeff              2    2 0.007 3.75  # c0 -
pair_coeff              3    3 0.0634 3.7584      # c2 -
pair_coeff              4    4 0.071 3.884 # c3 -
pair_coeff              5    5 0.0668 3.9147      # cp -
pair_coeff              6    6 0.85 4.1214 # Cs+ -
pair_coeff              7    7 0.023 2.878 # h -
pair_coeff              8    8 0.008 1.087 # h* -
pair_coeff              9    9 0.092 3.89  # nn -
```