## Quickstart Guide to Model Structures and Interactions of Artificial Molecular Muscles with Efficient Computational Methods

# Electronic Supplementary Information (ESI)

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### List of Abbreviations

AMM	Artificial Molecular Muscle
GFN	Geometries, Frequencies, Non-covalent interactions
$\mathbf{FF}$	Force Field
хТВ	extended Tight-Binding
$\mathrm{DFT}$	Density Functional Theory
DFT-D	Dispersion corrected Density Functional Theory
MD	Molecular Dynamics simulation
$\operatorname{SQM}$	Semiempirical Quantum Mechanical method
PMx	Parametric Method Version X
DFTB	Density Functional Tight-Binding
CREST	Conformer Rotamer Ensemble Sampling Tool
ALPB	Analytically generalized Poisson Boltzmann continuum solvation model
SPE	Single Point Energy
ESI	Electronic Supporting Information
NDI	Naphthalene diimide
$\operatorname{CR}$	Contraction Ratio
SIE	Self Interaction Error
$\mathrm{mRRHO}$	modified Rigid Rotor Harmonic Oscillator
COSMO-RS	Conductor-like Screening Model for Real Solvents
TZVP	Triple Zeta Valence Polarization
DFA	Density Functional Approximation
SASA	Solvent Accessible Solvent Area
SCF	Self Consistent Field
MSINDO	Modified Symmetric Orthogonalized Intermediate Neglect of Differential Overlap
OPLSAA	Optimized Potentials for Liquid Simulations for All Atoms
UFF	Universal Force Field
GAFF	Generalized Amber Force Field
CAESAR	Conformer Algorithm based on Energy Screening and Recursive Buildup
OM	Orthogonalization Methods
CPCM	conductor-like polarizable continuum model
GBSA	Generalized Born Surface Area
USPEX	Universal Structure Predictor: Evolutionary Xtallography
ABC	Artificial Bee Colony genetic algorithm

## **Additional Computational Details**

**xtb** was used as driver for MOPAC2016 Version 19.179L<sup>S1</sup> for the calculation of PM*x* energies. *Gibbs* free energies in solution were calculated according to  $\Delta G_{c-s} = \Delta E_{el} + \Delta G_{mRRHO}^{T}(+\Delta \delta G_{solv})$  whereas  $\Delta E_{el}$  is the electronic dispersion corrected energy on various theoretical levels,  $\Delta G_{mRRHO}^{T}$  is the modified rigid-rotor-harmonic-oscillator (mRRHO) contribution calculated on GFN2-xTB<sup>S2</sup> level of theory at 298 K using the biased Hessian approach (bhess), <sup>S3</sup> and  $\Delta \delta G_{solv}$  is the solvation free energy calculated with the implicit solvation model ALPB and with COSMO-RS<sup>S4</sup> on BP86/def-TZVP level of theory. As the PM*x* methods are parametrized to yield reaction enthalpies H, only the -T · S contribution of bhess was used for the calculation of  $\Delta G$ . The solvation corrections were throughout calculated in CHCl<sub>3</sub>, except for AMM 1 which was investigated in DMSO.<sup>S5</sup> The gas phase contraction free energy was calculated according to  $\Delta G_c = \Delta E_{el} + \Delta G_{mRRHO}^{T}$  without solvent contributions. In case of a erroneous SCF convergence of DFA single-point energies, orbitals from a converged calculation using a different DFA were used as starting point. This prevents direct comparison of computation timings in the respective cases as well as the parallelization on more than 4 CPUs.

The MD simulation was conducted in a canonical ensemble, the run time was set to 1 ns with a propagation step size of 1 ps, *Berendsen* thermostat was set to 298 K, the hydrogen mass was set to 2 a.u. at the GFN2-xTB and to 4 a.u. at the GFN-FF level, all bonds were constrained from breaking using the SHAKE algorithm. During MDs, constraints to the st-sl distances were applied to maintain the disentangled form but still allowing bending and slipping. The CRs were calculated using the probability weighted average st-st distances, whereby all distances with a occurrence smaller than 5% relative to the maximally occurring distance were neglected and the first 20% of trajectory length were cut off to exclude the equilibration phase from statistics.

The proposed workflow may in principle also be executed using other programs than CREST on GFN2-xTB(ALPB) level. Alternatives to xTB are the established PM6 or PM7 method, OM methods<sup>S6</sup>, MSINDO<sup>S7</sup> or classical FF like GAFF<sup>S8</sup>, OPLSAA<sup>S9</sup> or UFF<sup>S10</sup>. Other implicit solvent models are e.g. COSMO<sup>S4</sup>, GBSA<sup>S11</sup> or CPCM<sup>S12</sup>. The conformer search can also be conducted with methods like for example USPEX<sup>S13</sup>, ABC<sup>S14</sup>, simulated annealing or CAESAR<sup>S15</sup>.

### Additional Tables and Figures

In the following, supporting tables for applied distance constraints, single-point energy timings, additional relative contraction energies, absolute energies, statistical data of the distance distributions and the distance distributions themselves are displayed.

AMM	d(st-st)	d(st-sl)	d(sl-r)
$1_{long}$	144-329	4-144, 258-329	33-342, 63-271 89-340, 115-221
$1_{short}$	144-329	4-144, 258-329	$\begin{array}{c} 134-345, \ 152-225\\ 53-283, \ 6-223\end{array}$
$2_{long}$	178-325	2-178, 258-325	231-252, 232-420 3-276, 130-249
$2_{short}$	178-325	2-178, 258-325	220-437, 221-299 130-264, 231-254
$3_{long}$	12-314	314-430, 12-164	230-489, 410-489 238-480, 191-480
$3_{short}$	12-314	314-430, 12-164	315-490, 104-490 360-489, 235-489
$4_{long}$	147-285	285-366, 1-147	84-379, 85-330 5-376, 46-262
$4_{short}$	147-285	285-366, 1-147	63-290, 2-298 127-356, 122-309

Table S1: Applied distance constraints during structure generation and MDs using the numbering of the appended structures.

Table S2: CPU timings in seconds for single point energies at different theoretical levels, conducted in parallel on 4 CPUs of model Intel®Xeon®CPU E3-1270 v5 @ 3.60GHz. <sup>1</sup>): value not comparable to other data due to different parallelization and starting point.

	$1_{\mathrm{long}}$	$1_{ ext{short}}$	$2_{ ext{long}}$	$2_{ ext{short}}$	$3_{ ext{long}}$	$3_{ ext{short}}$
$r^2$ SCAN-3c	2823	3219	7033	7715	140953	_1)
$GFN1-xTB^{S16}$	12	12	14	14	55	61
GFN2-xTB	10	10	12	13	53	61
$\operatorname{GFN}\operatorname{-}\operatorname{FF}^{\operatorname{S17}}$	0.3	0.3	0.6	0.4	0.5	0.6
PM6-D3H4X	6	6	11	12	15	12
PM7	251	205	9	10	29	52

Table S3: Gas phase reaction *Gibbs* free energies  $(\Delta G_c)$  of several contraction reactions in kcal·mol<sup>-1</sup> calculated on additional levels of theory. All methods were calculated with the def2-TZVP basis set.

	$1_{long} \longrightarrow 1_{short}$	$2_{long} {\longrightarrow} 2_{short}$	$3_{long} \longrightarrow 3_{short}$
$\omega B97 X\text{-}V^{S18}$	22.9	-21.6	-241.2
$B3LYP-D4^{S19}$	23.3	-16.1	-231.7
$B3LYP-NL^{S20}$	22.6	-53.5	-248.8

Table S4: Reaction *Gibbs* free energies in solution  $(\Delta G_{c-s})$  of several contraction reactions in kcal  $\cdot$  mol<sup>-1</sup> calculated on different levels of theory with  $\Delta \delta G_{solv}$  from COSMO-RS.

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$1_{long} \longrightarrow 1_{short}$	$2_{long} {\longrightarrow} 2_{short}$	$3_{long} \longrightarrow 3_{short}$
-1.6	6.9	-553.1
-0.7	0.9	-546.9
-0.3	6.5	-537.4
-1.0	-30.9	-554.5
-1.4	7.8	-551.5
1.6	7.6	-498.0
-0.9	9.8	-521.0
-13.3	-16.7	-542.8
-38.2	-13.3	-565.5
0.2	10.6	-489.0
-3.0	6.6	-463.8
-28.2	-6.0	-471.5
	$\begin{array}{c} 1_{long} \longrightarrow 1_{short} \\ & -1.6 \\ & -0.7 \\ & -0.3 \\ & -1.0 \\ & -1.4 \\ & 1.6 \\ & -0.9 \\ & -13.3 \\ & -38.2 \\ & 0.2 \\ & -3.0 \\ & -28.2 \end{array}$	$\begin{array}{c cccc} 1_{long} & \longrightarrow & 1_{short} & 2_{long} & \longrightarrow & 2_{short} \\ \hline & -1.6 & 6.9 \\ & -0.7 & 0.9 \\ & -0.3 & 6.5 \\ & -1.0 & -30.9 \\ & -1.4 & 7.8 \\ & 1.6 & 7.6 \\ & -0.9 & 9.8 \\ & -13.3 & -16.7 \\ & -38.2 & -13.3 \\ & 0.2 & 10.6 \\ & -3.0 & 6.6 \\ & -28.2 & -6.0 \end{array}$

	$\mid 1_{long} \longrightarrow 1_{short}$	$2_{long} {\longrightarrow} 2_{short}$	$3_{long} {\longrightarrow} 3_{short}$
$\omega B97X-D4$	-14.8	-2.1	-221.2
$\omega B97X-V$	-14.0	-8.1	-215.1
B3LYP-D4	-13.6	-2.5	-205.6
B3LYP-NL	-14.3	-39.9	-222.7
PBE0-D4	-14.7	-1.2	-219.7
PBE-D4	-11.6	-1.3	-166.1
$r^2$ SCAN-3c	-14.1	0.8	-189.2
PM6-D3H4X	-26.5	-25.7	-211.0
PM7	-51.6	-22.2	-233.6
GFN2-xTB	-13.1	1.6	-157.2
GFN1-xTB	-16.3	-2.3	-132.0
GFN-FF	-41.4	-15.0	-139.6

Table S5: Reaction *Gibbs* free energies in solution  $(\Delta G_{c-s})$  of several contraction reactions in kcal · mol<sup>-1</sup> calculated on different levels of theory with  $\Delta \delta G_{solv}$  from ALPB.

Table S6: Absolute energies in Eh  $(E_{el})$  on different levels of theory using xtb V6.4.1 (as driver for MOPAC).

	$E_{el}$ / Eh						
AMM	PM6-D3H4X	PM7	GFN1-xTB	GFN2-xTB	GFN-FF		
$1_{\text{long}}$	-1.112160025951	-2.112870739555	-601.179958	-570.669568	-57.161583		
$1_{\rm short}$	-1.093055288427	-2.133595551742	-601.144725	-570.62923	-57.166361		
$2_{\text{long}}$	-3.650569691603	-3.904188305381	-801.974302	-753.844935	-76.120179		
$2_{\rm short}$	-3.723050292875	-3.971161034436	-802.010582	-753.874858	-76.176602		
$3_{\text{long}}$	1.562062250334	0.457503580849	-749.834777	-734.593872	-91.351477		
$3_{\rm short}$	1.194897092606	0.054247418063	-750.10231	-734.901645	-91.631258		

Table S7: Absolute energies in Eh  $(E_{el})$  on different levels of theory applying a def2-TZVP basis set wherever possible using TURBOMOLE V7.5.1.

	$E_{el}$ / Eh							
AMM	$\omega B97X$	$\omega B97X-V$	B3LYP-D4	PBE0-D4	PBE-D4	$r^2$ SCAN-3c		
$1_{\text{long}}$	-8733.227931	-8733.011357	-8731.061426	-8725.809757	-8725.272168	-8730.290759		
$1_{\rm short}$	-8733.189338	-8732.972414	-8731.021866	-8725.771941	-8725.229464	-8730.252063		
$2_{\text{long}}$	-11633.412718	-11633.163580	-11630.660760	-11623.655037	-11623.000085	-11629.546169		
$2_{\text{short}}$	-11633.428942	-11633.208963	-11630.697259	-11623.689463	-11623.034738	-11629.577358		
$3_{\text{long}}$	-14880.060056	-14879.660998	-14877.175900	-14869.943800	-14869.094125	-14876.508548		
$3_{\rm short}$	-14880.454042	-14880.061050	-14877.560811	-14870.351117	-14869.416139	-14876.867233		

Table S8: Absolute energies in Eh and kcal  $\cdot$  mol<sup>-1</sup> for different energy contributions. <sup>1</sup>): DMSO instead of CH<sub>3</sub>Cl.

AMM	$\begin{vmatrix} G_{mRRHO}^T / \text{Eh} \\ \text{GFN2-xTB}(298\text{K}) \end{vmatrix}$	$G_{solv}$ / Eh ALPB(CH <sub>3</sub> Cl)	$G_{solv} / \text{kcal} \cdot \text{mol}^{-1}$ COSMO-RS(CH <sub>3</sub> Cl)	$E_{disp}$ / Eh D4	$-T \cdot S / Eh$ GFN2-xTB(298 K)
$1_{\text{long}}$	2.818118	$-0590187448^{1)}$	$-327.214^{1)}$	-0.115014	-0.421368
$1_{\rm short}$	2.815688	$-0.648964^{1)}$	$-350.842^{1)}$	-0.116011	-0.424044
$2_{\text{long}}$	3.539885	-0.356676	-138.438	-0.182651	-0.525197
$2_{\rm short}$	3.550770	-0.335018	-115.888	-0.202246	-0.515336
$3_{\rm long}$	3.623274	-0.628557	-76.575	-0.166457	-0.500206
$3_{\rm short}$	3.638995	-0.587037	-382.347	-0.182260	-0.510782

	av. dist.	most prob. dist.	SD
$4_{long}$ (GFN2-xTB)	64.9	64.9	10.2
$4_{\text{long}}$ (GFN-FF)	63.4	63.4	20.0
$4_{\rm short}$ (GFN2-xTB)	41.9	41.6	10.1
$4_{\mathrm{short}}$ (GFN-FF)	42.2	43.2	21.5

Table S9: Statistical data of distance distributions derived from MDs under neglect of distance probabilities below 5% of the maximal probability. Average distances, the most probable distances and standard deviations (SD) are given in Å.

stopper-to-stopper distance / $\rm pm$	absolute probability / $\%$	stopper-to-stopper distance / pm	absolute probability / $\%$
6269	0 141181957	6659	0 345878421
6275	0.081735176	6665	0 388443074
6281	0	6671	0.091733848
6287	0	6677	0 160589914
6203	0.071629934	6683	0
6200	0.500157710	6680	0 121480634
6305	0.503107710	6605	0.121405034
6911	0.323121073	6701	0.185006226
6217	0.303418007	6707	0.183000330
0317	0.245120555	0707	0.000047580
0323	0.400077103	0713	0.194493686
0329	0.618102452		
0335	0.706939597		
6341	0.753013982		
6347	1.293048867		
6353	1.445103661		
6359	0.946523561		
6365	0.846544863		
6371	0.793239146		
6377	0.513971611		
6383	2.087710871		
6389	2.027127039		
6395	2.790245060		
6401	3.559293066		
6407	3.234311866		
6413	3.200176778		
6419	2.501690702		
6425	2.564043669		
6431	3.274975616		
6437	3.629205812		
6443	4.563754075		
6449	4.102334884		
6455	4.561424340		
6461	5.339871255		
6467	3.826474364		
6473	4.128280896		
6479	5.463818136		
6485	6.195438768		
6491	7 457726765		
6497	6.527786151		
6503	5 489291683		
6509	5 143577326		
6515	4 546541888		
6521	5 253803020		
6597	5 667807013		
6522	4 596959749		
6520	4.020000740		
0000 6545	4.019200097 1 058687167		
0040 6551	4.050007407		
0001 6557	4.3040/1340		
0007	4.012333247		
6563	3.560627868		
6575	2.618322586		
6581	3.338885053		
6587	1.909097085		
6593	2.118800612		
6599	1.380492313		
6605	1.060558610		
6611	0.903800286		
6617	1.243222419		
6623	1.202927044		
6629	1.708209507		
6635	0.620698306		
6641	0.575171507		
6647	0.290611235		
6653	0.106044581		
	1		1

Table S10: Probabilities in % of stopper-to-stopper distances in pm for the RDF of AMM  ${\bf 4}_{\rm long}$  at the GFN2-xTB(CH\_3Cl) level.

stopper-to-stopper distance / pm	absolute probability / $\%$	stopper-to-stopper distance / pm	absolute probability / $%$
4012.5	0.007363829	4332.5	0.8655608721
4017.5	0.264690794	4337.5	0.3280508855
4022.5	0.039498314	4342.5	0.6081145590
4027.5	0.231286786	1312.0	0.7992080066
4022.5	0.005080172	4259.5	0.4401715447
4032.5	0.005069175	4332.3	0.4491710447
4037.5	0.387542682	4357.5	0.3702331665
4042.5	0.556937918	4362.5	0.09203645302
4047.5	1.117878339	4367.5	0.1685684209
4052.5	0.445043418	4372.5	0.2996525791
4057.5	0.421509626	4377.5	0.2206293563
4062.5	0.803091431	4382.5	0
4067.5	1.105784709	4387.5	0.1699085048
4072.5	1.361139074	4392.5	0.2856181944
4077.5	2.465984834	4397.5	0
4082.5	2 178458030	4402.5	ů ů
4087.5	1.277400261	4407.5	0
4007.5	2.749417592	4407.5	0
4092.5	3.742417523	4412.5	0
4097.5	2.739753117	4417.5	0.2099941339
4102.5	3.039154834	4422.5	0.0149735133
4107.5	3.496847762	4427.5	0
4112.5	3.298837371	4432.5	0
4117.5	3.900250099	4437.5	0.0154168348
4122.5	3.259313125	4442.5	0.2070941612
4127.5	4.141494899		
4132.5	3 230301113		
4132.5	5.616670354		
4137.5	0.010079354 0.00010750		
4142.5	0.309210759		
4147.5	4.401443311		
4152.5	5.455943751		
4157.5	6.678266509		
4162.5	4.463100935		
4167.5	4.870342716		
4172.5	4.484095443		
4177.5	4.176905908		
4182.5	4 725709930		
4182.5	6 555778054		
4107.5	E 770E77647		
4192.5	5.779577647		
4197.5	5.101869647		
4202.5	3.237572638		
4207.5	4.844254477		
4212.5	3.985228739		
4217.5	5.269154280		
4222.5	5.143098873		
4227.5	3.560501807		
4232.5	5.152023407		
4237.5	3,925855301		
4242 5	4 152382555		
4947 S	4 180622108		
4241.0	4.103023100		
4252.5	3.493840905		
4257.5	3.868501303		
4262.5	2.787429740		
4267.5	2.912068866		
4272.5	2.331008181		
4277.5	2.598950644		
4282.5	3.700020511		
4287.5	3.245622680		
4202 5	2 630060268		
4202.0	2.00000200		
4201.0 4200 E	2.000027094		
4302.0	2.080007109		
4307.5	1.678294936		
4312.5	1.148202633		
4317.5	1.154469706		
4322.5	1.199787316		
4327.5	1.786228787		

Table S11: Probabilities in % of stopper-to-stopper distances in pm for the RDF of AMM  $4_{short}$  at the GFN2-xTB(CH<sub>3</sub>Cl) level.

594.5         0         638.5         2.73643196           534.5         0         6407.5         3.54165215           535.5         0         6416.5         3.878673175           5840.5         0.263233022         6443.5         3.57923004           5845.5         0.263383022         6443.5         3.51399230           5845.5         0.263383022         6443.5         3.51399230           5875.5         0.13834262         6425.3         3.41358541           5875.5         0         6417.5         2.2885530           5903.5         0         6417.5         2.2885500           5903.5         0.138547383         6485.5         2.2885500           5903.5         0.317451642         6506.5         1.55014406           5933.5         0.1230384         652.4         1.143789303           5933.5         0.1230384         652.4         0.314745159           5944.5         0.113010461         653.3         0.903832901           5945.5         0.1230384         652.4         0.31472713           5944.5         0.1230384         654.5         0.31472533           5947.5         0.33320292         6542.5         0.31472533	stopper-to-stopper distance $/$ pm	absolute probability / $\%$	stopper-to-stopper distance / pm	absolute probability / $\%$
5813.5         0         638.5         2.2534105           5831.5         0         6416.5         3.854105           5843.5         0.259527301         643.5         3.5706049651           5845.5         0.229527301         643.4         3.5706049651           5855.5         0.239527301         643.4         3.57339004           5857.5         0         6416.5         2.51349980           5857.5         0         6417.5         2.238358032           5853.5         0         6470.5         3.2126921           5853.5         0         6470.5         3.2349804           5893.5         0.315647363         6488.5         2.248858030           5993.5         0.31574642         6670.5         3.1249920           5993.5         0.1293384         6633.5         0.90832801           5993.5         0.1293384         6635.5         0.51151647           5964.5         0.15933868         6651.5         0.53151647           5964.5         0.15933868         6651.5         0.32089201           5964.5         0.15937488         6651.5         0.24142135           6042.5         0.15937488         6651.5         0.24142135	5804 5	0	6389.5	2 728671111
5822.5         0         6407.5         3.54126216           5840.5         0.0         6415.5         3.57637176           5840.5         0.20338032         6425.5         3.5130093           5858.5         0.20338032         643.5         3.5130093           5867.5         0.2238426         6452.5         3.41358841           5876.5         0.2238426         6452.5         3.41358841           588.5         0         6471.5         2.51449930           589.5         0.1567733         6407.5         2.6338303           591.5         0.2338033         6473.5         2.9383803           5921.5         0.37451642         6506.5         1.15501406           5939.5         0.123013584         6524.5         0.41451647           5948.5         0.123013584         6524.5         0.4156633           5975.5         0.33202092         6542.5         0.54156633           5985.5         0.123013584         6524.5         0.24157169           5985.5         0.23882201         5384.5         0.23882201           5985.5         0.2388263         6606.5         0.23882201           5985.5         0.23867758         0.241421135	5813.5	Ő	6398.5	2 505481995
331.5         0         6416.5         3.2769/3967176           5840.5         0.27957701         6434.5         3.70619661           5858.5         0.220577301         6443.5         3.56130003           587.5         0.12883426         6452.5         3.41356841           5875.5         0         6461.5         2.51349930           5885.5         0         6470.5         2.9326644           5891.5         0         6470.5         2.9236080           5903.5         0.15847583         6488.5         2.29830800           5912.5         0.317451642         6506.5         1.6702898           5921.5         0.317451642         6506.5         1.620288           5935.5         0.033302692         6542.5         0.51156477           5936.5         0.13389716         6551.5         0.51372653           5975.5         0.02387116         6595.5         0.23374160           5984.5         0.13887146         6551.5         0.21472135           6002.5         0.19856670         6587.5         0.2309186319           6022.5         0.230714160         6695.5         0.641415647           6023.5         0.2702013         6613.5         0	5822.5	0	6407.5	3 5/1265215
Skill 5         0         0         1425.5         3.75900.0610           S58.5         0.26338302         6443.5         3.759230041           S58.5         0.26338302         6443.5         3.55130093           S58.5         0         6461.5         2.51310930           S58.5         0         6470.5         3.21326610           S58.5         0         6470.5         2.2430375           S591.5         0.32550335         6488.5         2.24303875           S592.5         0.23550335         6487.5         1.61702898           S593.5         0.23550335         6497.5         1.61702898           S593.5         0.23250335         6497.5         1.616702898           S593.5         0.23230384         6621.5         1.14457159           S593.5         0.23384291         651.5         0.132883291           S593.5         0.2133848         6651.5         0.20387291           S593.5         0.2133848         6551.5         0.21372853           S593.5         0.159414133         6578.5         0.204142135           S693.5         0.195414133         6578.5         0.204142145           S693.5         0.195414133         6565.5	5022.0	0	6416 5	2 979672176
38.3.3         0.2.307200         0.42.3.3         3.371500030           3885.5         0.2.3083022         6443.5         3.371500030           5885.5         0.28838302         6443.5         3.371500030           5885.5         0.28838302         6447.5         3.241300030           5885.5         0         6470.5         3.231386140           5897.5         0.3584.5         0         6470.5         2.243003875           5912.5         0.2355033         6447.5         1.6702898           5921.5         0.337451612         6506.5         1.54501406           5939.5         0.123013584         6524.5         1.144587159           5945.5         0.1339191601         6533.5         0.51375653           5945.5         0.13393868         6551.5         0.51375653           5945.5         0.13393868         6565.5         0.51375653           5947.5         0.023412747         6560.5         0.230892201           5948.5         0.159451493         6677.5         0.230892201           5947.5         0.230871608         6605.5         0           5947.5         0.230892201         6587.5         0.2004973277           6947.5         0.27640838 </td <td>5651.5 E840 E</td> <td>0</td> <td>6495 5</td> <td>2 706040651</td>	5651.5 E840 E	0	6495 5	2 706040651
S848.3         0.20952/311         644.5         3.561250004           S858.3         0.202838420         642.3         3.451350031           S87.3         0         6441.5         2.31349900           S86.5         0         6470.5         2.21349061           S86.5         0         6470.5         2.2312206140           S903.5         0.32550335         6486.5         2.2312206140           S903.5         0.32550335         6486.5         2.2312206140           S930.5         0.23550335         6486.5         2.41702808           S930.5         0.23550335         6485.5         1.145114406           S930.5         0.13391051         6533.5         0.51372553           S966.5         0.13384716         6551.5         0.133847159           S967.5         0.02341247         6560.5         0.33082201           S984.5         0.15385710         6569.5         0.24142135           6002.5         0.207660135         6605.5         0.03082201           5984.5         0.138414193         6757.5         0.24142135           6002.5         0.207660135         6605.5         0.640432141           6022.5         0.2766033         6615.5	5840.5	0	0425.5	3.700049051
SSR.3         0.263383422         6443.3         3.413508341           SST6.5         0.26338422         6443.3         3.413508341           SST6.5         0         6471.3         2.31349930           SSR.5         0         0.1564733         6473.3         2.21349930           SSR.5         0.1564733         6473.5         2.9833803         6475.5         2.4772898           SSR.5         0.31741642         6506.5         1.15501400         5305.5         0.9833803           SSR.5         0.33741642         6506.5         1.03239830         5008.5         0.154300           SSR.5         0.333422092         6515.5         0.543563         0.44537150           SSR.5         0.1334322092         6542.5         0.5435663         0.302892201           SSR.5         0.023412747         6560.5         0.23394160         5993.5         0.23412747           SSR.5         0.023412747         6560.5         0.230892201         5994.5         0.154341433         6696.5         0.20374160           SSR.5         0.02412747         6560.5         0.230892201         5993.5         0.30146831           602.5         0.237671638         6596.5         0.203692201         5993.5	5849.5	0.259527301	6434.5	3.579230904
5867.5         0.122333269         6432.5         3.113568341           5876.5         0         6410.3         2.313206140           5885.5         0         6470.5         2.985368303           5943.5         0.1358475833         6488.5         2.244063875           5921.5         0.23563035         6487.5         1.0702808           5931.5         0.137451642         6566.5         1.14497180           5936.5         0.1291136011         6524.5         0.14497191           5966.5         0.0373202020         6542.5         0.515731           5967.5         0.023412747         6560.5         0.33726533           5975.5         0.0237116         6590.5         0.20374100           5984.5         0.153887116         6590.5         0.20374100           5983.5         0.159841193         6578.5         0.20374100           6020.5         0.20760138         66041.5         0.20374100           6020.5         0.20760138         66614.5         0.20374100           6020.5         0.20760138         66632.5         0           6020.5         0.20760138         66632.5         0           6047.5         0.3730574137         66614.5         <	5858.5	0.263383032	6443.5	3.561350093
5876.5         0         6401.5         2.31349930           5884.5         0         6470.5         3.232206140           5894.5         0.5547583         64488.5         2.248535030           5912.5         0.325503035         6497.5         1.41702898           3030.5         0.1251341         6504.5         1.14657159           3030.5         0.122013584         6524.5         1.14557159           3048.5         0.151901901         6533.3         0.00332291           3048.5         0.151901901         6533.5         0.0141276533           3045.5         0.02412747         6560.5         0.32082201           3045.5         0.02357160         6541.5         0.230571400           3045.5         0.02357160         6563.5         0.023571400           3045.5         0.133857168         6565.5         0.230571400           3045.5         0.1398768070         6537.5         0.230571400           3045.5         0.30760135         6661.5         0.20091603           6002.5         0.307762035         6661.5         0.20091603           6047.5         0.307762035         0         0           6047.5         0.3077521477         6641.5	5867.5	0.128383426	6452.5	3.413568341
5885.5         0         6470.5         2.323206140           5894.5         0.155547533         6488.5         2.23063875           5912.5         0.337451642         6506.5         1.4702898           5921.5         0.337451642         6506.5         1.140587150           5930.5         0.08807310         6515.5         1.142587150           5944.5         0.151901961         6553.5         0.03322652           5957.5         0.033202692         6542.5         0.51372653           5966.5         0.73338868         6551.5         0.03322637           5993.5         0.023412747         6560.5         0.230832291           5993.5         0.023412747         6560.5         0.230892201           5993.5         0.05981670         6567.5         0.230892201           5993.5         0.15941193         6578.5         0.241421135           6002.5         0.028715988         6566.5         0.0340831           6001.5         0.027640933         6641.5         0.044083194           6029.5         0.027640933         6641.5         0.044083194           6026.5         0.037074928         6623.5         0           60047.5         0.0370674137	5876.5	0	6461.5	2.513499930
5894.5         0         6479.5         2.28833803           5912.5         0.1255/17583         64188.5         2.24003375           5912.5         0.171451642         6506.5         1.1617028984           5921.5         0.0171451642         6506.5         1.14357159           5930.5         0.028307310         6515.5         1.14357159           5948.5         0.151901961         6533.5         0.03032291           5957.5         0.0233220292         6542.5         0.04157653           5965.5         0.0179338868         6551.5         0.03032291           5984.5         0.153887116         6569.5         0.202574160           5993.5         0.154887168         6660.5         0.208071408           6001.5         0.018939870         6567.5         0.202574160           6023.5         0.02760136         6603.5         0.2004180381           6020.5         0.20760136         6603.5         0.2004180381           6023.5         0.191457098         6632.5         0         0           6023.5         0.191457098         6632.5         0         0           6023.5         0.194157098         6632.5         0         0           6023.5<	5885.5	0	6470.5	3.213266140
5903.5         0.1584783         6488.5         2.243003875           5912.5         0.237451642         6606.5         1.15601400           5930.5         0.0830730         6515.5         1.1028098           5983.5         0.123013544         6524.5         0.1415719           5987.5         0.33202092         6642.5         0.5151647           5967.5         0.023412747         6560.5         0.230932201           5983.5         0.15941493         6578.5         0.230932201           5984.5         0.15941493         6578.5         0.23093201           6002.5         0.028412747         6560.5         0.02082201           6003.5         0.027660136         6665.5         0.030186381           6011.5         0.088715988         6566.5         0.000179227           6029.5         0.15941493         6623.5         0           6003.5         0.197469833         6641.5         0           60047.5         0.372762938         6623.5         0           6005.5         0.037571437         6661.5         0           6005.5         0.136949434         6668.5         0           6005.5         0.1375910398         6662.5         0	5894.5	0	6479.5	2.988358030
5912.5         0.337630035         6497.5         1.617028988           5500.5         0.54501406         515.5         1.10329803           5590.5         0.13201354         652.5         1.144587159           5598.5         0.151901961         6533.5         0.003832891           5596.5         0.33320269         6542.5         0.511456647           5596.5         0.179338806         650.1.5         0.5328573           5597.5         0.023412747         6500.5         0.23289201           5594.5         0.15981119         6509.5         0.203571460           5903.5         0.159811193         6577.5         0.201421135           6002.5         0.198571598         6509.5         0.03418214           6022.5         0.207660138         6605.5         0.20149227           6023.5         0.191457988         6632.5         0           60375.5         0.21668991         0         0           6035.5         0.1972712988         6663.5         0           6035.5         0.73072135         6663.5         0           6035.5         0.19351109         6695.5         0           6035.5         0.19351109         6695.5         0 <td>5903.5</td> <td>0.158547583</td> <td>6488.5</td> <td>2.243063875</td>	5903.5	0.158547583	6488.5	2.243063875
5321.5         0.317451642         6500.5         1.45014406           5330.5         0.12901354         6524.5         1.144587159           5395.5         0.151901961         6535.5         0.00382291           5397.5         0.33202092         6542.5         0.041516647           5967.5         0.023412747         6560.5         0.320802201           5981.5         0.153887116         6560.5         0.230802201           5981.5         0.153887116         6560.5         0.230802201           5981.5         0.153887116         6560.5         0.230802201           5981.5         0.15885670         6577.5         0.320802831           6002.5         0.27610833         6614.5         0.21566891           6020.5         0.27610833         6661.5         0.300183314           6020.5         0.277610833         6641.5         0.194579388           6038.5         0.194579388         6632.5         0           6065.5         0.277610833         6663.5         0           6065.5         0.27760938         6632.5         0           6065.5         0.19535419         6695.5         0           6062.5         0.195354194         6695.5	5912.5	0.235503035	6497.5	1.617028998
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	5921 5	0.317451642	6506.5	1 545014406
	5930 5	0.086307310	6515.5	1 103208303
3338.3         0.123013064         0524.3         1.14486129           3348.5         0.1519013961         6533.5         0.903832891           3367.5         0.33302692         6542.3         0.511316647           3566.5         0.17933868         6551.3         0.333209221           35975.5         0.02312747         6560.5         0.203574160           35983.5         0.15387116         6560.5         0.203574160           35935.5         0.159414193         6578.5         0.240571400           6002.5         0.20760136         6600.5         0.30018681           6011.5         0.08715988         6596.5         0.6040314           6025.5         0.2760933         6614.5         0           6047.5         0.37262938         6632.5         0           6045.5         0.27029155         6650.5         0         0           6056.5         0.27029155         6650.5         0         0           6055.5         0.20760136         66695.5         0         0           6055.5         0.2072713         6641.5         0         0           6105.5         0.185015882         6667.5         0         0           6110.5	5000.5 E020 E	0.102012594	6504 5	1.105256505
3948.3         0.101901901         033.3         0.938.3281           3966.3         0.17938868         6551.5         0.514516647           3966.3         0.13938868         6551.5         0.3372653           5984.5         0.159414193         6678.5         0.203874160           5993.5         0.159414193         6678.5         0.203874120           6002.5         0.19895670         6587.5         0.3001863314           6022.5         0.27660833         6614.5         0.21566891           6023.5         0.20760136         6605.5         0.004079227           6038.5         0.19457998         6623.5         0           6047.5         0.20729155         6650.5         0           6047.5         0.20728155         6650.5         0           6047.5         0.20728155         6650.5         0           6047.5         0.20728155         6650.5         0           6047.5         0.20728155         6650.5         0           6045.5         0.20728155         0         0           6074.5         0.20728155         0         0           6101.5         0.47554091         6668.5         0           6110.5	5959.5	0.123013384	0324.3	1.144087109
356.5         0.33202992         6.42.5         0.541104647           3566.5         0.17933868         6551.5         0.230892201           5984.5         0.153887116         6560.5         0.203574160           5993.5         0.159414193         6578.5         0.241421135           6002.5         0.19805670         6587.5         0.30018031           6011.5         0.085715988         6596.5         0.09408314           6020.5         0.20760136         6605.5         0.09403144           6020.5         0.21566891         0         0           6025.5         0.27609833         6614.5         0.21566891           6038.5         0.191457998         6623.5         0           6047.5         0.37276398         6632.5         0           6047.5         0.20702155         6650.5         0           6065.5         0.19457988         6668.5         0           6074.5         0.186949434         6665.5         0           6028.5         0.186949434         6665.5         0           6101.5         0.43276933         66865.5         0           6110.5         0.432766634         6695.5         0           6128.5<	5948.5	0.151901961	6533.5	0.903832891
5966.5         0.179338868         6651.5         0.53726553           5984.5         0.139847147         6660.5         0.230892201           5984.5         0.139847147         6660.5         0.230892201           5993.5         0.139414193         6677.5         0.241421135           6002.5         0.19955670         6587.5         0.300479227           6011.5         0.068715988         6696.5         0.004063144           6029.5         0.27660833         6614.5         0.215669911           6038.5         0.191377988         6623.5         0           6035.5         0.20702155         6650.5         0           6035.5         0.20702155         6650.5         0           6036.5         0.20702155         6650.5         0           6036.5         0.20702155         6650.5         0           6037.5         0.20702155         0         0           6038.5         0         0         0           6037.5         0.20702155         0         0           6038.5         0         0         0           6137.5         0.23719963         6668.5         0           6101.5         0.424521404	5957.5	0.333202692	6542.5	0.541516647
5975.5 $0.023412747$ $6560.5$ $0.232852201$ $5984.5$ $0.153887116$ $6578.5$ $0.241421135$ $6002.5$ $0.19805670$ $6578.5$ $0.241421135$ $6002.5$ $0.02675715988$ $6596.5$ $0.084083194$ $6020.5$ $0.207660136$ $6605.5$ $0.094079227$ $6029.5$ $0.27762038$ $6623.5$ $0.0717227$ $6036.5$ $0.37272938$ $6623.5$ $0$ $6047.5$ $0.37272938$ $6632.5$ $0$ $6065.5$ $0.207028155$ $6650.5$ $0$ $6065.5$ $0.207028155$ $6665.5$ $0$ $6065.5$ $0.2321929292$ $6667.5$ $0$ $6065.5$ $0.23219633$ $6666.5$ $0$ $6074.5$ $0.185049434$ $6668.5$ $0$ $6025.5$ $0.85915882$ $6677.5$ $0$ $6101.5$ $0.472524698$ $6695.5$ $0$ $6110.5$ $0.472524698$ $6695.5$ $0$ $6119.5$ $0.624266634$ $0$ $614.5$ $0.92787777$ $6137.5$ $0.840493753$ $6290.5$ $1.6073573$ $6295.73$ $6295.73$ $6297.5$ $1.28403753$ $6295.73$ $6235.5$ $6235.5$ $1.282493753$ $6235.5$ $1.282493753$ $6235.5$ $1.282493753$ $6235.5$ $1.282493753$ $6235.5$ $1.2856373$ $6235.5$ $1.282493753$ $6235.5$ $1.2856373$ $6235.5$ $2.550861511$ $6335.5$ $2.550861511$ $6335.5$ $2.560861511$ $6$	5966.5	0.179338868	6551.5	0.513726553
5984.5 $0.15341143$ $6578.5$ $0.243574160$ $6002.5$ $0.18965670$ $6587.5$ $0.24121135$ $6001.5$ $0.098575988$ $6596.5$ $0.090479227$ $6029.5$ $0.276409833$ $6614.5$ $0.215668991$ $6029.5$ $0.276409833$ $6614.5$ $0.215668991$ $6038.5$ $0.191457998$ $6623.5$ $0$ $6065.5$ $0.373674137$ $6661.5$ $0$ $6056.5$ $0.27022155$ $6650.5$ $0$ $6055.5$ $0.27022155$ $6650.5$ $0$ $6074.5$ $0.2732719633$ $6668.5$ $0$ $603.5$ $0.185018822$ $6677.5$ $0$ $610.5$ $0.327199633$ $6686.5$ $0$ $611.5$ $0.327199633$ $6686.5$ $0$ $611.5$ $0.327199633$ $6686.5$ $0$ $611.5$ $0.321462962$ $617.5$ $0$ $6146.5$ $0.53313794$ $6144.5$ $0.92787777$ $6173.5$ $0.484661322$ $617.5$ $1.229692373$ $6$	5975.5	0.023412747	6560.5	0.320892201
5993.5         0.139456670         6587.5         0.241421135           6002.5         0.139856670         6587.5         0.300156381           6023.5         0.207660136         6605.5         0.084083194           6029.5         0.2776409833         6614.5         0.20568991           6038.5         0.191457998         6623.5         0           6047.5         0.3727629383         6663.5         0           6065.5         0.20702155         6660.5         0           6065.5         0.20702155         6660.5         0           6065.5         0.20702155         6660.5         0           6074.5         0.18591582         6677.5         0           6083.5         0.18591582         6677.5         0           6101.5         0.47524698         6695.5         0           6110.5         0.47524698         6695.5         0           6110.5         0.47254698         6695.5         0           6128.5         0.43162902         6146.5         0.593473944           6135.5         1.142679273         5         1.28517981           6131.5         0.272426634         5         1           6236.5         1.6	5984.5	0.153887116	6569.5	0.203574160
6002.5         0.198058670         6587.5         0.330186381           6011.5         0.058715988         6506.5         0.03048314           6020.5         0.207660136         6605.5         0.090479227           6023.5         0.276409833         6614.5         0           6038.5         0.191457998         6623.5         0           6047.5         0.3730574137         6661.5         0           6055.5         0.207028155         6650.5         0           6074.5         0.193534109         6668.5         0           6035.5         0.185915882         6677.5         0           6035.5         0.185915882         6675.5         0           6035.5         0.185915882         6675.5         0           6101.5         0.32140233         6686.5         0           6110.5         0.47254698         6695.5         0           6110.5         0.62426634         -         -           6137.5         0.231462962         -         -           6146.5         0.93313944         -         -           6135.5         1.142679273         -         -           6145.5         0.58726070         -	5993.5	0.159414193	6578.5	0.241421135
6011.5         0.08715988         6596.5         0.084083194           6020.5         0.27660136         6605.5         0.090479227           6038.5         0.191467998         6623.5         0           6038.5         0.372762938         6632.5         0           6055.5         0.3730574137         6641.5         0           6065.5         0.370574137         6641.5         0           6074.5         0.195354109         6659.5         0           6074.5         0.195354109         6659.5         0           6083.5         0.185915882         6677.5         0           6092.5         0.185915882         6675.5         0           6101.5         0.327199633         6686.5         0           6110.5         0.472264998         6695.5         0           6110.5         0.472264998         6695.5         0           6137.5         0.231462962         6695.5         0           6145.5         1.142679273         6164.5         0.594473944           6155.5         1.142679273         6164.5         0.567426070           6200.5         1.028433753         6220.5         1.60376749           6224.5	6002.5	0.198958670	6587.5	0.390186381
6020.5         0.207600136         6605.5         0.090479227           6029.5         0.276409833         6614.5         0.215668991           6038.5         0.191487998         6632.5         0           6055.5         0.730571137         6641.5         0           6055.5         0.207028155         6650.5         0           6065.5         0.191487197         6661.5         0           6074.5         0.19535109         6659.5         0           6083.5         0.186919434         6668.5         0           6092.5         0.18591582         6677.5         0           6101.5         0.327199033         66685.5         0           6110.5         0.475254098         6695.5         0           6128.5         0.400109347         5         0           6137.5         0.231420962         5         1           6146.5         0.593473944         5         5           6145.5         0.59347394         5         5           6137.5         0.434661322         5         1.69276749           6131.5         0.567420070         5         5         5           6205.5         1.69263673	6011.5	0.085715988	6596.5	0.084083194
6029.5         0.276409833         6614.5         0.215668991           6038.5         0.191457998         6623.5         0           6065.5         0.372762938         6663.5         0           6065.5         0.3730574137         6641.5         0           6065.5         0.20708155         6665.5         0           6074.5         0.195354109         6655.5         0           6074.5         0.18691434         6668.5         0           6092.5         0.18691434         6668.5         0           6101.5         0.327199633         66685.5         0           6110.5         0.473254098         6695.5         0           6110.5         0.624266634	6020.5	0 207660136	6605.5	0.090479227
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0.003.3 $0.12747/3238$ $0.023.3$ $0.023.3$ $0.047.5$ $0.372762938$ $0.6632.5$ $0.16632.5$ $0.16632.5$ $0.0665.5$ $0.207028155$ $6650.5$ $0.16632.5$ $0.16632.5$ $0.074.5$ $0.195354109$ $6659.5$ $0.16632.5$ $0.16632.5$ $0.083.5$ $0.186949434$ $6668.5$ $0.1610.5$ $0.327199633$ $6686.5$ $0.1610.5$ $0.101.5$ $0.327199633$ $6686.5$ $0.1610.5$ $0.475254698$ $6695.5$ $0.1610.5$ $0.110.5$ $0.475254698$ $6695.5$ $0.1610.5$ $0.2214629634$ $1.1627.5$ $0.1611.5$ $0.110.5$ $0.231462962$ $0.161.5$ $0.1619273$ $1.126277.5$ $0.1611.5$ $0.110.5$ $0.231462962$ $0.164.5$ $0.92787777$ $0.173.5$ $0.484661322$ $0.161.5$ $0.15217981$ $0.163756749$ $0.163756749$ $0.200.5$ $1.028433753$ $0.227.5$ $1.228015474$ $0.205.5$ $1.639230031$ $0.245.5$ $0.238904275$ $0.227.5$ $1.283015474$ $0.238504275$ $0.238904275$ $0.290.5$ $2.500661511$ $0.33058867$ $0.299.5$ $0.290.5$ $2.500661511$ $0.3335.5$ $4.046456488$ $0.343.5$ $0.238947926$ $0.23852100$ $0.23892477926$ $0.325.5$ $2.892477926$ $0.289247926$ $0.289247926$ $0.335.5$ $0.26099836$ $0.2609836$ $0.2609836$	6038 5	0.101457008	6623.5	0.21000391
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	6065.5	0.207028155	6650.5	0
	6074.5	0.195354109	6659.5	0
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6182.5 $1.155217981$ $6191.5$ $0.567426070$ $6200.5$ $1.028433753$ $6209.5$ $1.603756749$ $6218.5$ $1.529693573$ $6227.5$ $1.283015474$ $6236.5$ $1.639230031$ $6245.5$ $1.828649387$ $6254.5$ $1.478634455$ $6263.5$ $2.858851549$ $6272.5$ $2.175913567$ $6281.5$ $2.58904275$ $6290.5$ $3.300588567$ $6290.5$ $2.5006615111$ $6308.5$ $2.520195036$ $6317.5$ $2.512100904$ $6335.5$ $4.046456488$ $6344.5$ $3.634390111$ $6353.5$ $2.892477926$ $6371.5$ $3.260909836$	6173.5	0.484661322		
6191.5 $0.567426070$ $6200.5$ $1.028433753$ $6209.5$ $1.603756749$ $6218.5$ $1.529693573$ $6227.5$ $1.283015474$ $6236.5$ $1.639230031$ $6245.5$ $1.828649387$ $6254.5$ $1.828649387$ $6254.5$ $2.85851549$ $6263.5$ $2.85851549$ $6272.5$ $2.175913567$ $6281.5$ $2.538904275$ $6290.5$ $3.300588567$ $6299.5$ $2.560661511$ $6308.5$ $2.520195036$ $6317.5$ $2.1910904$ $6326.5$ $2.896517860$ $6335.5$ $4.046456488$ $6344.5$ $3.634390111$ $6335.5$ $2.6897822$ $6362.5$ $2.892477926$ $6371.5$ $3.726352100$ $6380.5$ $3.260909836$	6182.5	1.155217981		
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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	6227.5	1.283015474		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	6236.5	1.639230031		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	6245 5	1.828649387		
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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	6272.5	2.175913567		
6290.5       3.300588567         6299.5       2.560661511         6308.5       2.520195036         6317.5       2.512100904         6326.5       2.896517860         6335.5       4.046456488         6344.5       3.634390111         6353.5       2.665897822         6362.5       2.892477926         6371.5       3.726352100         6380.5       3.260909836	6281.5	2.538904275		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	6290.5	3.300588567		
6308.5       2.520195036         6317.5       2.512100904         6326.5       2.896517860         6335.5       4.046456488         6344.5       3.634390111         6353.5       2.665897822         6362.5       2.892477926         6371.5       3.726352100         6380.5       3.260909836	6299.5	2.560661511		
	6308.5	2.520195036		
6326.5       2.896517860         6335.5       4.046456488         6344.5       3.634390111         6353.5       2.665897822         6362.5       2.892477926         6371.5       3.726352100         6380.5       3.260909836	6317.5	2.512100904		
$      \begin{array}{ccccccccccccccccccccccccccccccc$	6326.5	2.896517860		
6344.5       3.634390111         6353.5       2.665897822         6362.5       2.892477926         6371.5       3.726352100         6380.5       3.260909836	6335.5	4.046456488		
6353.5     2.665897822       6362.5     2.892477926       6371.5     3.726352100       6380.5     3.260909836	6344.5	3.634390111		
6362.5     2.892477926       6371.5     3.726352100       6380.5     3.260909836	6353 5	2 665807822		
6332.5         2.832477920           6371.5         3.726352100           6380.5         3.260909836	6369 K	2.000031022		
03/1.5         3.720352100           6380.5         3.260909836	0002.0	2.092411920		
0380.0 3.200909830	03/1.5	3.720352100		
	6380.5	3.260909836		

Table S12: Probabilities in % of stopper-to-stopper distances in pm for the RDF of AMM  $$4_{\rm long}$$  at the GFN-FF(CH\_3Cl) level.

stopper-to-stopper distance / $\rm pm$	absolute probability / $\%$	stopper-to-stopper distance / pm	absolute probability / $\%$
3803.5	0	4258.5	2.134888780
3810.5	0	4265.5	2.636668651
3817.5	0	4272.5	2.384521874
3824.5	0	4279.5	2.047609157
3831.5	0	4286.5	2.653515540
3838.5	0	4293.5	2.722544306
3845.5	0	4300.5	3.475889831
3852.5	0.043033074	4307.5	4.245537497
3859.5	0.170741076	4314.5	4.130707082
3866.5	0.161148446	4321.5	4.678503527
3873.5	0.051510288	4328.5	3.251742389
3880.5	0.205733302	4335.5	3.512054349
3887.5	0.005559009	4342.5	3.968556939
3894.5	0.00000000	4349.5	3.202819578
3901.5	0.020531078	4356.5	4.390374877
3908.5	0.605802241	4363.5	4 053949006
3915 5	0.572243342	4370.5	3 230099135
3022.5	0.558719632	4377.5	2 053522158
3020.5	0.522339415	4384.5	2.000022100
2026 5	0.402207492	4901.5	2.255257455
3930.3	0.433337403 0.471501272	4331.5	1 808206577
2050 S	0.471301372	4030.0	0.000180776
3990.9 2057 5	0.000001147	4400.0 4410 5	1 156102077
3937.3 2064 F	0.277099924	4412.5	1.130103077
3904.3 2071 F	0.700404908	4419.5	1.079012084
3971.3 2078 F	0.703877390	4420.0	0.379330812
3978.3 2005 F	0.308392020	4455.5	0.320733219
3960.0 2000 F	0.775552918	4440.5	0.317909908
3992.5	1.009825371	4447.5	0.105445895
3999.5	0.919201592	4404.0	0.064509606
4000.3	0.802171770	4401.3	0.159501995
4015.5	0.418730900	4408.3	0.000555800
4020.5	1.141020040	4475.5	0
4027.5	1.557216727	4462.0	0
4034.5	1.006204407	4409.0	0
4041.5	1.230330147	4490.0	0
4048.5	1.822981889		
4055.5	1.792240002 1.756520218		
4062.5	1.750525218		
4005.5	1.017590341		
4070.5	1 310038231		
4090.5	2 249495983		
4097 5	2.01072202		
4104 5	1 944556347		
4111 5	2.335247714		
4118 5	2.053552068		
4125.5	1.862942336		
4132.5	1.544368000		
4139.5	2.259113230		
4146.5	2,600280674		
4153.5	1.435486592		
4160.5	1 709119191		
4167.5	2 025201281		
4174 5	1 892854801		
4181.5	1.878474501		
4188.5	1 912459281		
4195.5	1.009936438		
4202.5	1 779716524		
4209.5	2.321300018		
4216 5	2.063798400		
4223 5	2.556651611		
4230.5	2.557883782		
4237.5	2.299958262		
4244.5	1.225740995		
4251.5	1.482578094		
	1.102010001	1	

Table S13: Probabilities in % of stopper-to-stopper distances in pm for the RDF of AMM  ${\bf 4}_{\rm short}$  at the GFN-FF(CH\_3Cl) level.

#### References

- (S1) J. J. Stewart, J. Comput. Aided Mol. Des., 1990, 4, 1–103.
- (S2) C. Bannwarth, S. Ehlert and S. Grimme, J. Chem. Theor. Comput., 2019, 15, 1652– 1671.
- (S3) S. Spicher and S. Grimme, J. Chem. Theor. Comput., 2021, 17, 1701–1714.
- (S4) A. Klamt, Comput. Mol. Science, 2011, 1, 699–709.
- (S5) R. E. Dawson, S. F. Lincoln and C. J. Easton, Chem. Commun., 2008, 3980–3982.
- (S6) P. O. Dral, X. Wu, L. Sporkel, A. Koslowski, W. Weber, R. Steiger, M. Scholten and W. Thiel, J. Chem. Theor. Comput., 2016, 12, 1082–1096.
- (S7) T. Bredow, G. Geudtner and K. Jug, J. Comput. Chem., 2001, 22, 861–887.
- (S8) J. Wang, R. M. Wolf, J. W. Caldwell, P. A. Kollman and D. A. Case, J. Comput. Chem., 2004, 25, 1157–1174.
- (S9) G. A. Kaminski, R. A. Friesner, J. Tirado-Rives and W. L. Jorgensen, J. Phys. Chem. B, 2001, 105, 6474–6487.
- (S10) A. K. Rappé, C. J. Casewit, K. Colwell, W. A. Goddard III and W. M. Skiff, J. Am. Chem. Soc., 1992, 114, 10024–10035.
- (S11) J. Zhu, Y. Shi and H. Liu, J. Phys. Chem. B, 2002, 106, 4844–4853.
- (S12) Y. Takano and K. Houk, J. Chem. Theor. Comput., 2005, 1, 70–77.
- (S13) C. W. Glass, A. R. Oganov and N. Hansen, Comp. Phys. Comm., 2006, 175, 713–720.
- (S14) D. Karaboga and B. Basturk, J. Glob. Optim., 2007, **39**, 459–471.
- (S15) J. Li, T. Ehlers, J. Sutter, S. Varma-O'Brien and J. Kirchmair, J. Chem. Inf. Model., 2007, 47, 1923–1932.
- (S16) S. Grimme, C. Bannwarth and P. Shushkov, J. Chem. Theory Comput., 2017, 13, 1989–2009.
- (S17) S. Spicher and S. Grimme, Angew. Chem., 2020, 132, 15795–15803.
- (S18) N. Mardirossian and M. Head-Gordon, Phys. Chem. Chem. Phys., 2014, 16, 9904– 9924.
- (S19) J.-D. Chai and M. Head-Gordon, Phys. Chem. Chem. Phys., 2008, 10, 6615–6620.
- (S20) O. A. Vydrov and T. Van Voorhis, J. Chem. Phys., 2010, 133, 244103.