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[1] Molecule data were obtained from the authors of *White et al.* 1993 [3].

Table I : CH_3 Ω calculation using double overlap only, for all permutations

Calculation details[2]	Ω running total in steradians
Addition of all two atom solid angles:	
+ $\Omega_{(C\text{-}H1)}$:[1.460833]	= 1.460833
+ $\Omega_{(C\text{-}H2)}$:[1.460861]	= 2.921694
+ $\Omega_{(C\text{-}H3)}$:[1.460859]	= 4.382553
+ $\Omega_{(H1\text{-}H2)}$:[1.919629]	= 6.302182
+ $\Omega_{(H1\text{-}H3)}$:[1.919634]	= 8.221816
+ $\Omega_{(H2\text{-}H3)}$:[1.926091]	= 10.147907
Removal of all extra single atom solid angles:	
- 2*$\Omega_{(C)}$: [0.841767]	= 8.464373
- 2*$\Omega_{(H1)}$: [1.055183]	= 6.354007
- 2*$\Omega_{(H2)}$: [1.055183]	= 4.243640
- 2*$\Omega_{(H3)}$: [1.055180]	= 2.133280
Total solid angle for CH_3	= **2.133280sr** (97.327deg or 17% sphere)

[2] The numerical integration procedure was set to integrate to an accuracy of 10^{-6} and therefore all results have been given to six decimal places.

Table II : CH_3 Ω calculation using double overlap only, for select permutations (*White et al.*)

Calculation details	Ω running total in steradians
Addition of all two atom solid angles:	
+ $\Omega_{(C\text{-}H1)}$:[1.460833]	= 1.460833
+ $\Omega_{(C\text{-}H2)}$:[1.460861]	= 2.921694
+ $\Omega_{(C\text{-}H3)}$:[1.460859]	= 4.382553
Removal of extra single atom solid angles:	
- 2*$\Omega_{(C)}$: [0.841767]	= 2.699020
Total solid angle for CH_3	= **2.69902sr** (110.44deg or 21% sphere)

Table III : CH_3 Ω calculation using all orders of multiple overlap

Calculation details	Ω running total in steradians
Calculation of all single atom solid angles	
+ $\Omega_{(C)}$: [0.841767]	= 0.841767
+ $\Omega_{(H1)}$: [1.055183]	= 1.896950
+ $\Omega_{(H2)}$: [1.055183]	= 2.952133
+ $\Omega_{(H3)}$: [1.055180]	= 4.007313
Removal of all double overlaps	
- $\Omega_{(C\text{-}H1)}$:[0.436117]	= 3.571196
- $\Omega_{(C\text{-}H2)}$:[0.436090]	= 3.135106
- $\Omega_{(C\text{-}H3)}$:[0.436088]	= 2.699018
- $\Omega_{(H1\text{-}H2)}$):[0.190737]	= 2.508281
- $\Omega_{(H1\text{-}H3)}$):[0.190729]	= 2.317552
- $\Omega_{(H2\text{-}H3)}$):[0.184272]	= 2.133280
Addition of all triple overlaps	
+ $\Omega_{(H2\text{-}C\text{-}H1)}$ [0.170066]	= 2.303345
+ $\Omega_{(H3\text{-}C\text{-}H1)}$ [0.170061]	= 2.473407
+ $\Omega_{(H3\text{-}C\text{-}H2)}$ [0.166343]	= 2.639749
+ $\Omega_{(H3\text{-}H1\text{-}H2)}$ [0.039941]	= 2.679690
Removal of all quadruple overlaps	
- $\Omega_{(H3\text{-}H2\text{-}C\text{-}H1)}$ [0.039941]	= 2.639749
Total solid angle for CH_3	= **2.63975sr** (109.12deg or 21% sphere)

Table IV : Solid Angles and Cone Angles for 12 molecular fragments[3]

	Cone angle in radians	Solid angles in steradians[4]	
Fragment Name	Tolman procedure[5]	White et al.[6]	Multiple Overlap
Imidazole	1.491077	1.590351	1.415416
NH_2OH	1.742570	1.876093	1.685321
NH_3	1.789398	1.948819	1.859953
NH_2Me	1.982452	2.696721	2.322253
NH_2EtOH	2.002485	2.868522	2.326860
NH_2Me_3OH	2.046896	2.853271	2.537361
$NH_2Pr(OH)_2$	2.051723	2.988734	2.184162
PF_3	2.169660	2.609292	2.599425
PBr_3	2.472132	3.156167	3.154727
PEt_3	2.663106	4.122755	3.433989
PBz_3	3.000215	5.088678	4.221555
$P(C_6F_5)_3$	3.216643	4.673923	4.017541

[3] Molecule data were obtained from the authors of *White et al.* 1993 [3].

[4] The solid angles and cone angles are not in the same units, although it is a simple matter to convert from one to the other using equation 2, or to give them in terms of fractions of complete spheres or circles respectively.

[5] These values were calculated from the same molecular data as the solid angle measurements.

[6] These values were calculated from the same molecular data as the multiple overlap calculation, but using the algorithm described by *White et al.* 1993. [3]