

The Tetrahedral Stereocentre from Packing: Chirality’s Geometric Origin without Hybridisation

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Abstract

Molecular chirality rests on one geometric fact: a carbon centre is tetrahedral, so four distinct substituents admit two arrangements that are mirror images and not superimposable. That fact was inferred from optical activity in 1874, half a century before quantum mechanics, and the orbital account recovers it by *hybridising* one *s* and three *p* eigenmodes into four equivalent lobes — a construction laid over an independent-particle approximation, undertaken because the bare eigenmodes do not give molecular shape. We note that RealQM, a model of non-overlapping unit electron charge densities in three space dimensions, obtains the tetrahedron directly: four unit charges on a shell sit as far apart as the shell allows, and for $N = 4$ that is tetrahedral. The arrangement this has to beat is not a smeared shell but *square planar*, which is real chemistry — Pt(II), Pd(II), Ni(II) — and which is *achiral*, since a square’s own plane is a mirror plane: $3.674/R$ tetrahedral against $3.828/R$ square, a margin of 4.2%, on which the whole of stereochemistry rests. We are explicit that this margin is point-charge electrostatics – the $N = 4$ Thomson problem, and VSEPR’s argument quantified – not an output of the model. The calculation that is: four extended non-overlapping densities with kinetic energy on an isotropic kernel, free interfaces, seeded lopsidedly, relax into the tetrahedral basin and not the square one — standard deviation of the six angles 6–12° against 42.4° for square planar — though with a residual 8° short of regular that survives halving the cell size. The stereocentre is then a packing result rather than an orbital repair, and the existence of chirality follows from how charge packs around a kernel. We are equally explicit about what this does not deliver. Enantiomers come out exactly degenerate, which is correct but automatic in any parity-symmetric theory and therefore buys nothing. Enantioselectivity does not come out at all: a 95:5 enantiomeric ratio corresponds to $\Delta\Delta G^\ddagger \approx 1.7$ kcal/mol, three orders of magnitude below this model’s accuracy floor. Chiral recognition energies are typically under 1 kcal/mol and dispersion-dominated, which is a permanent gap. And the origin of biological homochirality requires parity violation, which the framework does not contain. The contribution is therefore to chirality’s *geometric origin*, not to chiral chemistry.

1 One geometric fact

Handedness is in the news: the 2026 Nobel Prize in Chemistry has gone to work on left- and right-handed molecules. This article is not about what such a prize is given for. Enantioselectivity and chiral recognition are quantitative questions about small energy differences, and

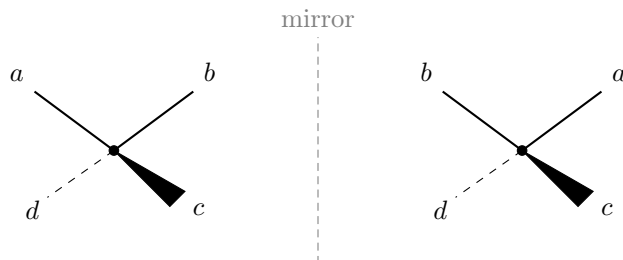


Figure 1: The whole of carbon chirality in one picture. A four-coordinate centre is tetrahedral; with four distinct substituents there are exactly two arrangements, related by reflection and not superimposable by any rotation. Bold wedge toward the reader, dashed away. Everything downstream — optical rotation, enantiomeric excess, the handedness of sugars and amino acids — rests on this.

Section 5 sets out why they lie one to three orders of magnitude beyond the model discussed here. It is about the fact underneath them, which is geometric rather than energetic — why a four-coordinate centre is tetrahedral at all, and so why handedness exists to be resolved, catalysed or awarded.

Chirality in carbon chemistry reduces to a single statement about shape. A centre bonded to four groups is tetrahedral; if the four groups differ, there are exactly two ways to arrange them, and the two are mirror images that cannot be brought into coincidence by any rotation. Everything else — optical rotation, enantiomeric excess, the handedness of sugars and amino acids — is built on that.

The historical order is worth keeping in view, because it is the reverse of the usual telling. Chemistry’s interest in handedness is older than quantum mechanics and older than the electron: Pasteur separated the two forms of tartrate by hand in 1848 [1] and Kelvin gave the property its name [2]. Van’t Hoff and Le Bel proposed the tetrahedral carbon in 1874 *in order to explain optical activity* [3, 4]. The tetrahedron was an empirical inference from chirality, not a prediction about it, and it preceded Schrödinger’s equation by fifty-two years. Quantum mechanics inherited the tetrahedron as something to be recovered.

2 How the orbital account recovers it

The one-electron hydrogenic states are s , p , d , f , classified by angular momentum. For carbon the occupied valence modes are one $2s$ and three $2p$, and the $2p$ lobes point along three mutually orthogonal axes. That is not a tetrahedron; orthogonal axes give 90° between bonds, where methane has 109.47° . The repair is *hybridisation*: one forms four linear combinations

$$\frac{1}{2}(s + p_x + p_y + p_z), \quad \frac{1}{2}(s + p_x - p_y - p_z), \quad \text{and two more,}$$

each pointing at a cube corner, and the four together are tetrahedral [7]. VSEPR does the same work by a different route, positing that electron pairs repel and arrange themselves at maximum separation [8].

Neither device is in the Schrödinger equation [6]. The N -electron equation has no orbitals at all; its solutions are functions on $3N$ variables carrying no s, p, d, f labels. The orbital scheme is an independent-particle approximation laid over it, and hybridisation is a further construction

laid over that, undertaken — as the companion article on atoms puts it — because “the bare eigenmodes do not give molecular shape.” VSEPR and sp^3 hybridisation are geometric repairs grafted onto the orbital model precisely to recover a shape the decomposition had destroyed.

This is not an objection to the orbital account, which is enormously useful and which we do not dispute. It is an observation about where the tetrahedron comes from in that account: it is put back in, by hand, after an angular decomposition removed it.

3 How packing gives it directly

RealQM carries no angular decomposition to undo. The state is a set of non-overlapping unit charge densities, and the question of where four charges sit on a shell is answered by minimising Coulomb repulsion subject to non-overlap. The answer is the obvious one: as far apart as the shell allows — antipodal for two, trigonal for three, **tetrahedral for four**.

The numbers make the point quantitative. For unit charges at a common radius R , in units of $1/R$:

charges	smeared over the shell	packed
2	1.000	0.500 (antipodal)
3	3.000	1.732 (trigonal)
4	6.000	3.674 (tetrahedral)

The same rule gives the shell capacities of the periodic table, where the closed octet appears as $8 = 4+4$, two dual tetrahedra, and where no s , p or d enters the construction anywhere.

The alternative that matters is not a smear

Beating a smeared shell by 63% is not much of a test, because nothing in chemistry is a smeared shell. The arrangement the tetrahedron has to beat is **square planar** — four charges on a great circle — and that one is real: platinum(II), palladium(II) and nickel(II) adopt it routinely, and it is the geometry that makes cisplatin work [10]. Four unit charges at radius R , all six pairs counted:

$$\begin{aligned} \text{square planar: } & 4 \times \frac{1}{R\sqrt{2}} + 2 \times \frac{1}{2R} = 3.828/R \\ \text{tetrahedral: } & 6 \times \frac{1}{2R \sin(109.47^\circ/2)} = \mathbf{3.674}/R \end{aligned}$$

The tetrahedron wins, but only by **4.2%**.

What that arithmetic is, and is not. It must be said plainly, because the number is easy to over-read. Both figures are six pairwise Coulomb terms between four *point* charges held at a fixed radius in two prescribed geometries. There is no kinetic energy in them, no extended density, no non-overlap constraint, no free boundary and no solver. This is the $N = 4$ Thomson problem [5] restricted to two candidates — arithmetic available since 1904, and identical in any theory that contains Coulomb repulsion. It is, in particular, exactly VSEPR’s own argument made quantitative: pairs repel, so they go tetrahedral. So the comparison establishes that *Coulomb repulsion favours the tetrahedron*, which was never in doubt, and it does *not* establish that this model derives the tetrahedron in any way the orbital account does not.

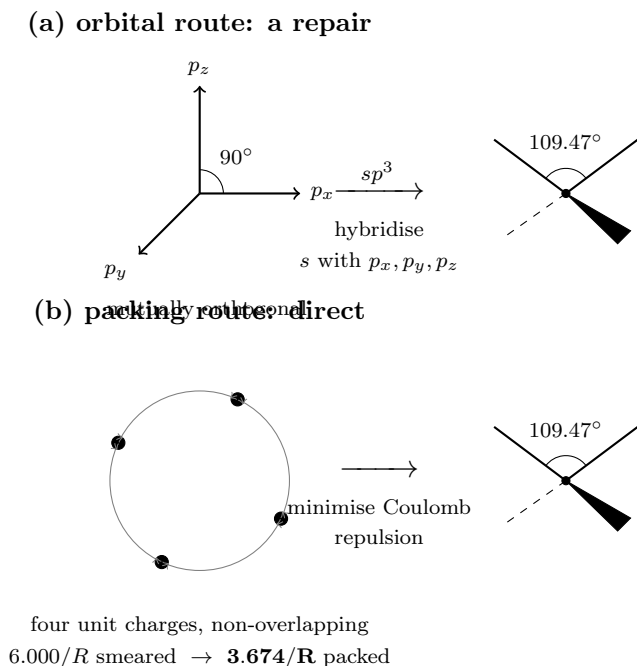


Figure 2: Two routes to the same tetrahedron. **(a)** The orbital account begins with three mutually orthogonal p lobes at 90° — not a tetrahedron — and recovers 109.47° by hybridising them with s . The shape is restored after an angular decomposition removed it. **(b)** RealQM takes no such decomposition: four non-overlapping unit charges on a shell minimise their mutual repulsion by sitting tetrahedrally. The energies shown are point-charge arithmetic at fixed radius — the $N = 4$ Thomson problem — and so belong to Coulomb repulsion generally rather than to this model; what distinguishes (b) from (a) is that no angular decomposition was taken and none has to be repaired, not the numbers.

The calculation that would distinguish the two accounts is a different one: four non-overlapping *extended* densities on a $+4$ kernel, carrying kinetic energy, with free interfaces and no angular structure imposed — solved, and asked where they settle when started from an arrangement that is neither tetrahedral nor square. We have run it, and report it in Section 4 with its limits.

That margin is the whole of stereochemistry, because **square-planar four-coordination is achiral**. Four distinct substituents on a square give *cis* and *trans* isomers, not enantiomers: the plane of the square is itself a mirror plane. The tetrahedron is the only four-coordinate geometry with no such plane. So optical activity, enantiomeric excess, the handedness of sugars and amino acids — all of it rests on four unit charges preferring the tetrahedron to the square by four per cent of their mutual repulsion. Had the square won for carbon, there would be no enantiomers to resolve and no chirality to award a prize for.

Even the ordering, then, is claimed as electrostatics rather than as this model’s output, and the margin is claimed not at all: whether RealQM reproduces 4.2% to better than itself is a question its few-per-cent accuracy floor on total energies does not let us answer. The ordering is what chirality requires and the margin is what selectivity would require, and Section 5 says why the second is out of reach.

So the stereocentre is a packing result. Chirality exists because four unit charges pack tetrahedrally around a kernel, and a tetrahedron with four distinct corners is chiral. No hybridisation is required because nothing was decomposed into orbitals in the first place. Of the two classical repairs, VSEPR is much the closer in spirit — it is a repulsion-and-separation argument, and RealQM is in effect VSEPR promoted from a rule to a solved variational problem.

4 What four densities actually do

Four unit charge densities are placed on an isotropic +4 point kernel, non-overlapping, with a common inner radius $r_c = 0.5$ a.u. — common, and therefore radial only, so it can express no angular preference. The interfaces are *free*: nothing fixes the partition, and the solver is able to relocate a domain. The seed is deliberately lopsided, each of the four directions rotated away from tetrahedral in alternating senses so that no symmetry is left for the relaxation to preserve. What is then measured is the *charge* centroid of each domain — $\int \rho \mathbf{r}$ over the cells of that label, divided by $\int \rho$ — and the six mutual angles between those four directions. Each domain’s charge integrates to 1.00, which is the check that the measurement is of what it claims.

box (a.u.)	seed	max dev. from 109.47°	range	s.d.
12	25° skew	9.8°	17.8°	6.1°
6	25° skew	8.2°	14.9°	5.9°
12	40° skew	19.9°	29.0°	11.9°
<i>regular tetrahedron</i>		0	0	0
<i>square planar</i>		70.5°	90°	42.4°

The arrangement lands unambiguously in the tetrahedral basin and not the square one: a standard deviation of 6–12° against 42.4° for square planar. That ordering is the model’s own output, obtained from extended densities carrying kinetic energy under a free partition, and it is the statement the chirality argument needs. It is not the same statement as the Thomson arithmetic above, which any Coulomb theory supplies.

Two limits must go with it. The relaxation does not reach the *regular* tetrahedron — a residual departure of about 8° remains — and the residual retains a memory of the seed, 8–10° from a 25° skew against 20° from a 40° skew, so these are not a unique minimum. And the residual is *not* a resolution artefact: halving the cell size, by running the same seed in a box of 6 instead of 12 a.u. at fixed grid, moved it only from 9.8° to 8.2°. We had expected refinement to collapse it and it did not, so the offset is algorithmic or physical rather than numerical, and we do not know which.

So what the model delivers here is the *ordering* — tetrahedral over square-planar, by a wide margin, from its own densities — and not the regular tetrahedron. Since chirality requires only that the four-coordinate arrangement be the tetrahedron rather than the square, the ordering is the part stereochemistry rests on; an 8° residual does not make a stereocentre achiral.

5 What this does not deliver

The above is a claim about the *origin* of chirality and nothing more. Four limits should be stated plainly, because each of them excludes something a reader might reasonably hope for.

Enantiomer degeneracy is automatic, and therefore worthless as evidence. Two enantiomers have exactly equal energy in any parity-symmetric theory. RealQM is Coulomb-only and hence parity-symmetric, so the degeneracy comes out exactly — and so it does in standard quantum mechanics. Nothing is learned either way.

Enantioselectivity is out of reach by three orders of magnitude. Selectivity is a transition-state energy difference. A 95:5 enantiomeric ratio at room temperature corresponds to $\Delta\Delta G^\ddagger \approx 1.7$ kcal/mol. This model’s energies are accurate to a few per cent of a total energy, which for an organic molecule is hundreds of kcal/mol. The gap is not a matter of refinement.

Chiral recognition energies lie in the dispersion gap. Discrimination between enantiomers by a chiral host is typically under 1 kcal/mol and is substantially dispersive. RealQM’s densities are static, so it has no dispersion; the same limitation that keeps it out of van der Waals complexes keeps it out of recognition thermodynamics. What it *can* address is the shape question — whether an enantiomer geometrically fits a pocket — since hydrogen-bond and steric geometries come out at measured distances. Whether it fits, not how much it prefers to.

Homochirality requires physics the framework lacks. That life uses L-amino acids and D-sugars is a broken symmetry, and breaking it requires parity violation — the weak interaction [11]. RealQM contains Coulomb interaction and nothing else. The origin of biological handedness is outside it, and no amount of computation changes that.

6 What is worth saying, then

Exactly one thing, and it is upstream of chiral chemistry rather than part of it. The founding geometric fact of stereochemistry — that a four-coordinate centre is tetrahedral — is in the orbital account a repair applied after an angular decomposition, and in RealQM a direct consequence of four non-overlapping charges minimising their mutual repulsion. Chirality is then a packing phenomenon: it exists because charge packs tetrahedrally, and a tetrahedron with four distinct corners has no mirror symmetry.

Van’t Hoff and Le Bel inferred the tetrahedron from optical activity in 1874. Pauling supplied hybridisation in 1931 to recover it from the new mechanics [7]. The claim here is that a model built from charge densities in three dimensions does not need the second step, because it never takes the decomposition that made it necessary.

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