

# IUCrJ

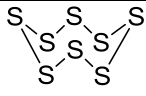
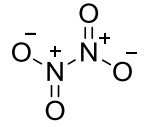
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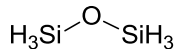
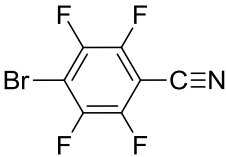
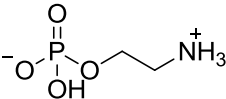
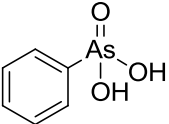


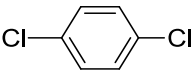
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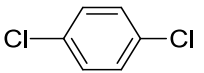
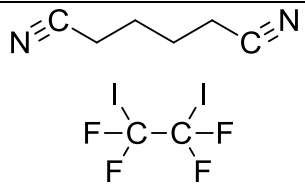
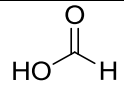
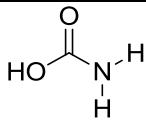
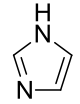
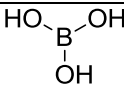
***CrystalExplorer* model energies and energy frameworks: extension to metal coordination compounds, organic salts, solvates and open-shell systems**

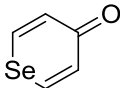
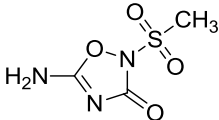
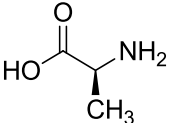
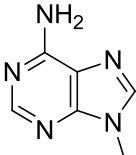
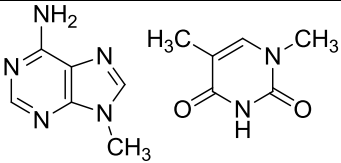
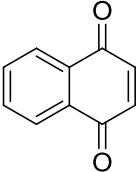
**Campbell F. Mackenzie, Peter R. Spackman, Dylan Jayatilaka and Mark A. Spackman**

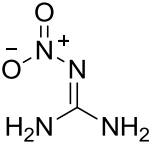
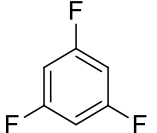
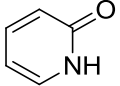
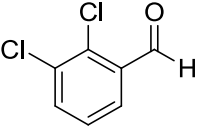
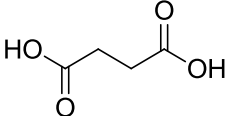
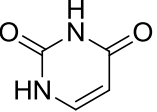
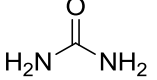
**Table S1****Table S2** Crystal structure details for 37 “neutral pairs”.


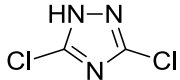
	Name	Diagram	Reference
15318- ICSD-I2	iodine	I—I	F. van Bolhuis, P.B. Koster, T. Migchelsen, <i>Acta Cryst.</i> (1967) <b>23</b> , 90.
200455- ICSD-S8	sulfur		P. Coppens, Y.W. Yang, R.H. Blessing, W.F. Cooper, F.K. Larsen, <i>J. Am. Chem. Society</i> (1977) <b>99</b> , 760.
201142- ICSD-N2O4	dinitrogen tetroxide		A. Kvick, R.K. McMullan, M.D. Newton, <i>J. Chem. Phys.</i> (1982) <b>76</b> , 3754.
201693- ICSD-Br2	bromine	Br—Br	B.M. Powell, K.M. Heal, B.H. Torrie, <i>Mol. Phys.</i> (1984) <b>53</b> , 929.
201698- ICSD-Cl2	chlorine	Cl—Cl	B.M. Powell, K.M. Heal, B.H. Torrie, <i>Mol. Phys.</i> (1984) <b>53</b> , 929.
260950- ICSD-XeF2	xenon difluoride	F—Xe—F	H.S.A. Elliot, J.F. Lehmann, H.P.A. Mercier, H.D.B. Jenkins, G.J. Schrobilgen, <i>Inorg. Chem.</i> (2010) <b>49</b> , 8504.

30501- ICSD- disiloxane	disiloxane		M.J. Barrow, E.A.V. Ebsworth, M.M. Harding, <i>Acta Cryst. B</i> (1979) <b>35</b> , 2093.
ACETYL02	acetylene	$\text{H}-\text{C}\equiv\text{C}-\text{H}$	R.K. McMullan, A. Kvik, P. Popelier, <i>Acta Crystallogr., Sect. B: Struct. Sci.</i> (1992), <b>48</b> , 726.
ACOKEI	4-bromo-2,3,5,6- fluorobenzonitrile		A.D. Bond, J. Griffiths, J.M. Rawson, J. Hulliger, <i>Chem. Commun.</i> (2001), 2488.
AEPHOS02	phosphorylethanolamine		H.-P. Weber, R.K. McMullan, S. Swaminathan, B.M. Craven, <i>Acta Crystallogr., Sect. B: Struct. Sci.</i> (1984), <b>40</b> , 506.
ARSACP02	phenylarsonic acid		N.C. Lloyd, H.W. Morgan, B.K. Nicholson, R.S. Ronimus, <i>J. Organomet. Chem.</i> (2008), <b>693</b> , 2443.
BENZEN01	benzene		G.E. Bacon, N.A. Curry, S.A. Wilson, <i>Proc. R. Soc. London, Ser. A</i> (1964), <b>279</b> , 98.
DCLBEN03 -gamma	p-dichlorobenzene		G.L. Wheeler, S.D. Colson, <i>Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem.</i> (1975), <b>31</b> , 911.
DCLBEN06 -beta	p-dichlorobenzene		G.L. Wheeler, S.D. Colson, <i>J. Chem. Phys.</i> (1976), <b>65</b> , 1227.

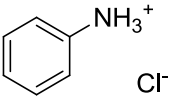
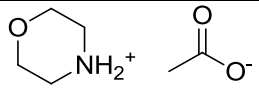
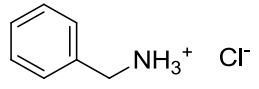
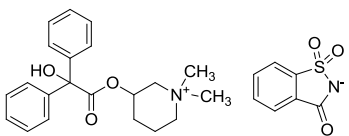
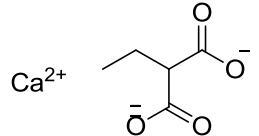
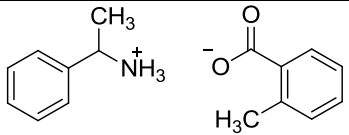
DCLBEN07 -alpha	p-dichlorobenzene		G.L.Wheeler, S.D.Colson, <i>J.Chem.Phys.</i> (1976), <b>65</b> , 1227.
EBIHIH	1,4-dicyanobutane 1,2-di-iodo- 1,1,2,2-tetrafluoroethane		P.Metrangolo, T.Pilati, G.Resnati, A.Stevenazzi, <i>Chem.Commun.</i> (2004), 1492.
ETHANE01	ethane	$\text{H}_3\text{C}-\text{CH}_3$	G.J.H.van Nes, A.Vos, <i>Acta Crystallogr., Sect.B: Struct. Crystallogr. Cryst. Chem.</i> (1978), <b>34</b> , 1947.
ETHLEN10	ethylene	$\text{H}_2\text{C}=\text{CH}_2$	G.J.H.van Nes, A.Vos, <i>Acta Crystallogr., Sect.B: Struct. Crystallogr. Cryst. Chem.</i> (1979), <b>35</b> , 2593.
FORMAC01	formic acid		I.Nahringbauer, <i>Acta Crystallogr., Sect.B: Struct. Crystallogr. Cryst. Chem.</i> (1978), <b>34</b> , 315.
FORMAM0 2	formamide		E.D.Stevens, <i>Acta Crystallogr., Sect.B: Struct. Crystallogr. Cryst. Chem.</i> (1978), <b>34</b> , 544.
IMAZOL13	imidazole		B.M.Craven, R.K.McMullan, J.D.Bell, H.C.Freeman, <i>Acta Crystallogr., Sect.B: Struct. Crystallogr. Cryst. Chem.</i> (1977), <b>33</b> , 2585.
JAGREP	orthoboric acid		R.R.Shuvalov, P.C.Burns, <i>Acta Crystallogr., Sect.C: Cryst. Struct. Commun.</i> (2003), <b>59</b> , i47.

JOYHUA	4H-selenopyran-4-one		M.R.Detty, H.R.Luss, <i>Organometallics</i> (1992), <b>11</b> , 2157.
JUPPAL	5-amino-2-mesy1-2,3-dihydro-1,2,4-oxadiazol-3-one		Do Young Ra, Nam Sook Cho, Sung Kwon Kang, Eun Suk Choi, Il Hwan Suh, <i>J.Chem.Soc.,Perkin Trans.2</i> (1999), 81.
LALNIN03	L-alanine		R.Destro, R.E.Marsh, R.Bianchi, <i>J.Phys.Chem.</i> (1988), <b>92</b> , 966.
MEADEN05	9-methyladenine		K.N.Jarzembska, A.M.Goral, R.Gajda, P.M.Dominiak, <i>Cryst.Growth Des.</i> (2013), <b>13</b> , 239.
MTHMAD1 1	9-methyladenine-1-methylthymine complex		M.N.Frey, T.F.Koetzle, M.S.Lehmann, W.C.Hamilton, <i>J.Chem.Phys.</i> (1973), <b>59</b> , 915.
NAPHQU	1,4-naphthoquinone		J.Gaultier, C.Hauw, <i>Acta Crystallogr.</i> (1965), <b>18</b> , 179.

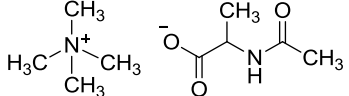
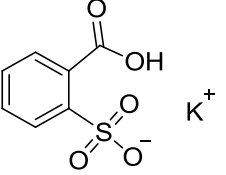
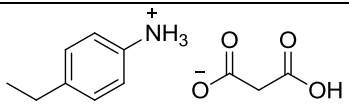
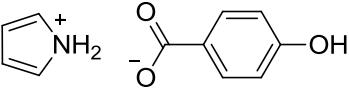
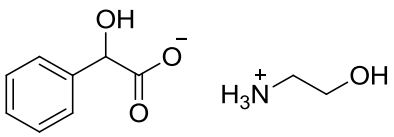
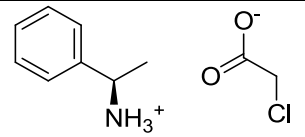
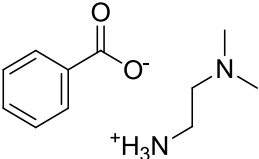
NTRGUA03	2-nitroguanidine		R.K.Murmann, R.Glaser, C.L.Barnes, <i>J.Chem.Cryst.</i> (2005), <b>35</b> , 317.
PVVAWA0 1	1,3,5-trifluorobenzene		V.R.Thalladi, H.-C.Weiss, D.Blaser, R.Boese, A.Nangia, G.R.Desiraju, <i>J.Am.Chem.Soc.</i> (1998), <b>120</b> , 8702.
PYRIDO04	2-pyridone		U.Ohms, H.Guth, E.Hellner, H.Dannohl, A.Schweig, <i>Z.Kristallogr.</i> (1984), <b>169</b> , 185.
QEWXIA01	2,3-dichlorobenzaldehyde		K.A.Solanko, A.D.Bondy, <i>Acta Crystallogr., Sect.B: Struct.Sci.</i> (2011), <b>67</b> , 437.
SUCACB09	1,4-butanedioic acid		V.R.Thalladi, M.Nusse, R.Boese, <i>J.Am.Chem.Soc.</i> (2000), <b>122</b> , 9227.
URACIL	uracil		R.F.Stewart, L.H.Jensen, <i>Acta Crystallogr.</i> (1967), <b>23</b> , 1102.
UREAXX12	urea		S.Swaminathan, B.M.Craven, R.K.McMullan, <i>Acta Crystallogr., Sect.B: Struct.Sci.</i> (1984), <b>40</b> , 300.

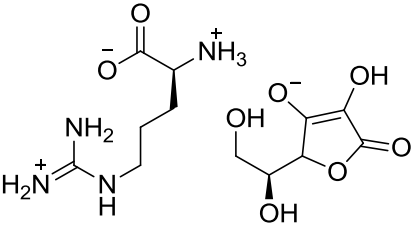
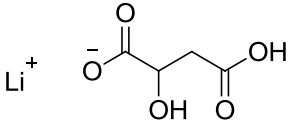
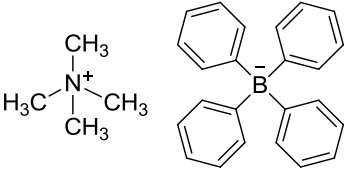
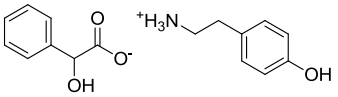
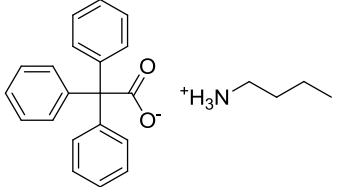
VAMZIT01	pentacyclo[4.4.0.0 <sup>2,5</sup> .0 <sup>3,8</sup> .0 <sup>4,7</sup> ]dec-9-ene (basketene)		S.P.Verevkin, M.Kummerlin, E.Hickl, H.-D.Beckhaus, C.Ruchardt, S.I.Kozhushkov, R.Haag, R.Boese, J.Benet-Bucholz, K.Nordhoff, A.de Meijere, <i>Eur.J.Org.Chem.</i> (2002), 2280.
VITRUL	3,5-dichloro-1H-1,2,4-triazole		G.L.Starova, O.V.Frank-Kamenetskaya, V.V.Makarskii, <i>Kristallografiya(Russ.)(Crystallogr.Rep.)</i> (1990), <b>35</b> , 769

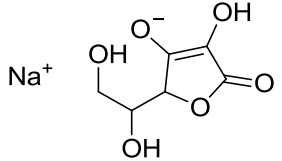
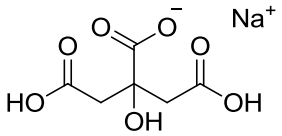
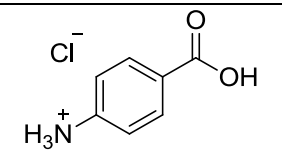
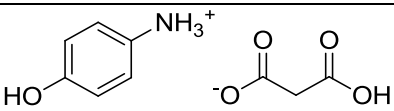
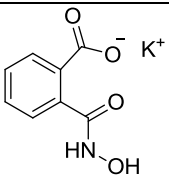
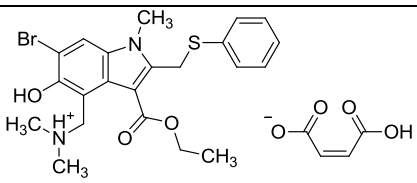
**Table S3** Crystal structure details for 44 organic salts, including solvates.

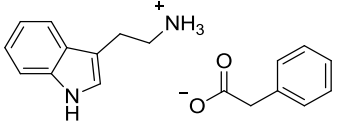
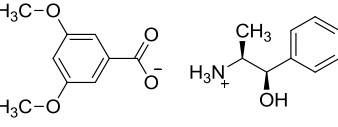
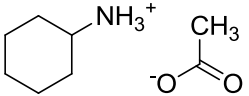
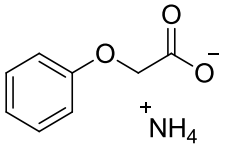
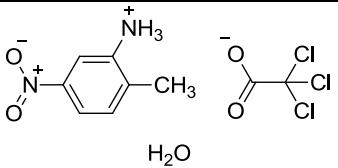
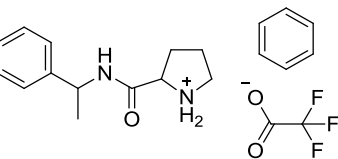
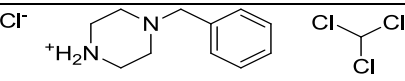
ANLINC01	anilinium chloride		E.Lopez-Dupla, P.G.Jones, F.Vancea, <i>Z.Naturforsch.,B:Chem.Sci.</i> (2003).
BEPTUN	morpholin-4-ium acetate		S.P.Kelley, A.Narita, J.D.Holbrey, K.D.Green, W.M.Reichert, R.D.Rogers, <i>Cryst.Growth Des.</i> (2013), <b>13</b> , 965.
BOGCAC	benzylammonium chloride		M.Topper, M.L.McLaughlin, F.R.Fronczek, <i>CSD Communication(Private Communication)</i>
COXYIY	3-(2-hydroxy(diphenyl)acetoxy)- 1,1-dimethylpiperidinium 3-oxo- 3H-1,2-benzothiazol-2-ide 1,1- dioxide  (mepenzolate saccharinate)		P.M.Dean, J.Turanjanin, M.Yoshizawa-Fujita, D.R.MacFarlane, J.L.Scott, <i>Cryst.Growth Des.</i> (2009), <b>9</b> , 1137.
CUZHEK	calcium $\alpha$ -ethylmalonate		A.Zell, H.Einspahr, C.E.Bugg, <i>Biochemistry</i> (1985), <b>24</b> , 533.
DEZYEO	1-phenylethanaminium 2- methylbenzoate		T.Sasaki, I.Hisaki, T.Miyano, N.Tohnai, K.Morimoto, H.Sato, S.Tsuzuki, M.Miyata, <i>Nat.Commun.</i> (2013), <b>4</b> , 1787.

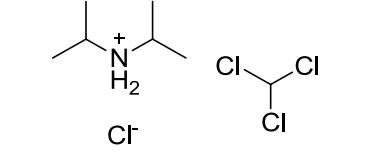
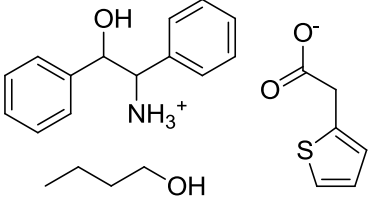
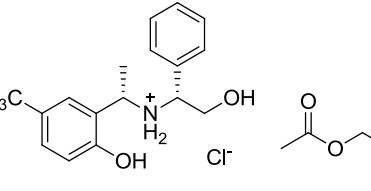
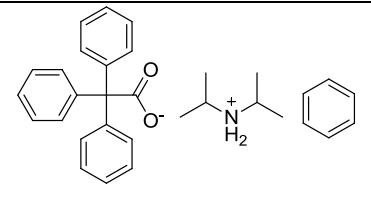
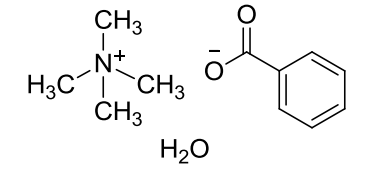


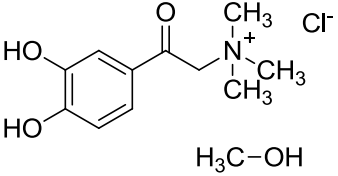
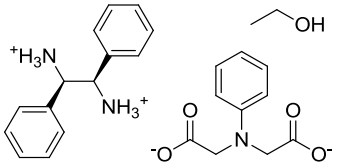
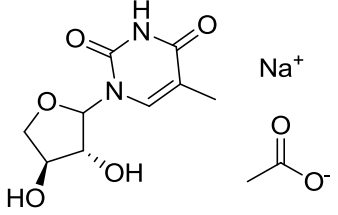
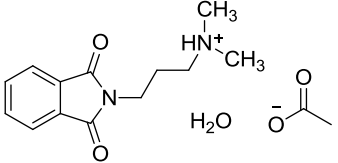
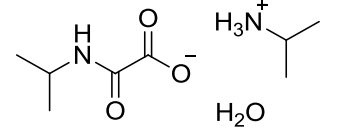
DUBWAZ	tetramethylammonium 2-(acetylamino)propanoate		T.Gelbrich, E.Shepherd, M.B.Hursthouse, J.D.Kilburn, <i>University of Southampton, Crystal Structure Report Archive</i> (2000), 405.
DUFBIP	potassium o-sulfonatobenzoic acid		T.B.Teplova, T.N.Turskaya, T.A.Shibanova, Yu.V.Nekrasov, G.S.Belikova, <i>Kristallografiya(Russ.)(Crystallogr.Rep.)</i> (1986), <b>31</b> , 187.
DUVCAZ	4-ethylanilinium 2-carboxyacetate		De-Hong Wu, Qi-Qi Wu, <i>Acta Crystallogr., Sect. E: Struct. Rep. Online</i> (2010), <b>66</b> , o2160.
FENYEC	pyrrolidinium p-hydroxybenzoate		Y.Moritani, N.Sasahara, S.Kashino, M.Haisa, <i>Acta Crystallogr., Sect. C: Cryst. Struct. Commun.</i> (1987), <b>43</b> , 154.
HEZXAM	2-hydroxyethanaminium (S)-hydroxy(phenyl)acetate (ethanolammonium mandelate)		N.Wermester, E.Aubin, M.Pauchet, S.Coste, G.Coquerel, <i>Tetrahedron: Asymm.</i> (2007), <b>18</b> , 821.
HISREG	(R)-(+)-1 phenylethylammonium chloroacetate		S.Houllemare-Druot, G.Coquerel, <i>J.Chem.Soc., Perkin Trans.2</i> (1998), 2211.
KUDFIA	2-(dimethylamino)ethanaminium benzoate		Dittrich, Dennis, Wolper, Christoph, Schulz, Stephan, <i>CSD Communication (Private Communication)</i>

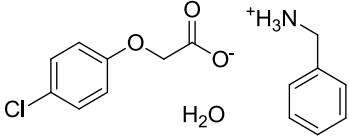
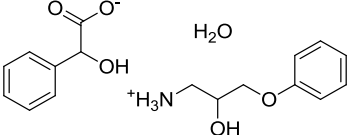
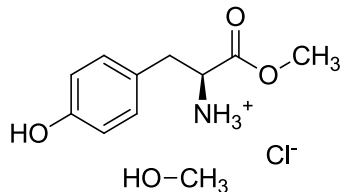
LARASC20	L-arginine L-ascorbate		V.Sudhakar, M.Vijayan, <i>Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem.</i> (1980), <b>36</b> , 120.
LIHMAM	lithium hydrogen (+)-1-malate		W.Van Havere, A.T.H.Lenstra, <i>Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem.</i> (1980), <b>36</b> , 1483.
MATPHB	tetramethylammonium tetraphenylborate		K.Hoffmann, E.Weiss, <i>J.Organomet.Chem.</i> (1974), <b>67</b> , 221.
MEDHOU 1	2-(4-hydroxyphenyl)ethanaminium hydroxy(phenyl)acetate		N.E.B.Briggs, A.R.Kennedy, C.A.Morrison, <i>Acta Crystallogr., Sect. B: Struct. Sci.</i> (2012), <b>68</b> , 453.
MIBTOH	n-butylammonium triphenylacetate		T.Yuge, N.Tohnai, T.Fukuda, I.Hisaki, M.Miyata, <i>Chem.-Eur.J.</i> (2007), <b>13</b> , 4163.

NAASCB	sodium ascorbate		J.Hvoslef, <i>Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem.</i> (1969), <b>25</b> , 2214.
NAHCIT	sodium dihydrogen citrate		J.P.Glusker, D.van der Helm, W.E.Love, M.L.Dornberg, J.A.Minkin, C.K.Johnson, A.L.Patterson, <i>Acta Crystallogr.</i> (1965), <b>19</b> , 561.
PAMBZA03	4-carboxyanilinium chloride		Wen Wu, Jiming Xie, Dongpo Xie, <i>Zh.Neorg.Khim.(Russ.)(Russ.J.Inorg.Chem.)</i> (2010), <b>55</b> , 384.
PAXNIN	4-hydroxyanilinium carboxylate		Ying-Chun Wang, <i>Acta Crystallogr., Sect. E: Struct. Rep. Online</i> (2012), <b>68</b> , o1937.
RIRMUA	potassium phthalohydroxamate		Z.Ch.Kadyrova, N.K.Makhmudova, Kh.T.Sharipov, N.A.Parpiiev, <i>Uzb.Khim.Zh.(Russ.)(Uzbek Journal on Chemistry)</i> (1996), 11-5.
SIYSEA	umifenovir hydrogen maleate		L.Orola, I.Sarcevic, A.Kons, A.Actins, M.V.Veidis, <i>J.Mol.Struct.</i> (2014), <b>1056</b> , 63.

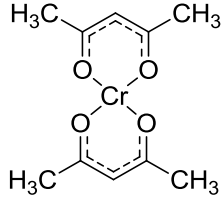
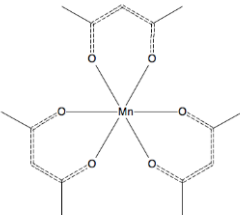
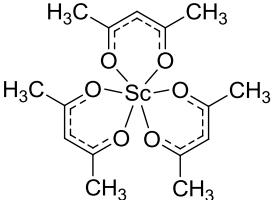
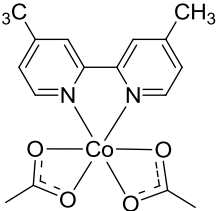
TRPPAC	tryptammonium phenylacetate		M.Inoue, T.Sakaki, T.Fujiwara, K.Tomita, <i>Bull.Chem.Soc.Jpn.</i> (1978), <b>51</b> , 1123.
TUYKAB	(1R,2S)-norephedrine 3,5-dimethoxybenzoate		Chunji Li, J.Cho, K.Yamada, D.Hashizume, F.Araoka, H.Takezoe, T.Aida, Y.Ishida, <i>Nat.Commun.</i> (2015), <b>6</b> , 8418.
YABFOY	cyclohexylammonium acetate		J.A.Odendal, J.C.Bruce, K.R.Koch, D.A.Haynes, <i>CrystEngComm</i> (2010), <b>12</b> , 2398,
ZOWWEP	ammonium phenoxyacetate		G.Smith, <i>Acta Crystallogr.,Sect.E:Struct.Rep.Online</i> (2014), <b>70</b> , 528,
FOVCAV	2-methyl-5-nitroanilinium trichloroacetate monohydrate		J.Janczak, G.J.Perpetuo, <i>Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.</i> (2009), <b>65</b> , o339.
GELSUM	(2S,1'R)-2-(1'-phenylethylcarbamoyl)pyrrolidinium trifluoroacetate benzene solvate		S.S.Chimni, D.Mahajan, <i>Tetrahedron:Asymm.</i> (2006), <b>17</b> , 2108.
HODPUM	4-benzylpiperazin-1-ium chloride chloroform solvate		M.G.Nema, R.A.Varga, C.Silvestru, H.J.Breunig, <i>Acta Crystallogr.,Sect.E:Struct.Rep.Online</i> (2008), <b>64</b> , o1585.

HORVAL	di-isopropylammonium chloride chloroform solvate		M.Nieger, E.Niecke, A.Loew, <i>CSD Communication(Private Communication)</i> (1999)
HURMOX	2-hydroxy-1,2-diphenylethanaminium 2-thienylacetate butan-1-ol solvate		N.Shiota, T.Kinuta, T.Sato, R.Kuroda, Y.Matsubara, Y.Imai, <i>Tetrahedron</i> (2010), <b>66</b> , 5589.
IDOPAT	N-((S)-1-(5-methyl-2-hydroxyphenyl)ethyl)-N-((R)-2-hydroxy-1-phenylethyl)amine chloride ethyl acetate solvate		Guang-You Zhang, Xiang-Bo Wang, Jin-Yan Zhao, Wan-Hui Wang, Xiao-Feng Yang, <i>Acta Crystallogr., Sect. E: Struct. Rep. Online</i> (2006), <b>62</b> , o3035.
IRURAO	diisopropylammonium triphenylacetate benzene solvate		K.Sada, T.Watanabe, J.Miyamoto, T.Fukuda, N.Tohnai, M.Miyata, T.Kitayama, K.Maehara, K.Ute, <i>Chem.Lett.</i> (2004), <b>33</b> , 160.
ISIHIB	tetramethylammonium benzoate monohydrate		H.-Stoekli-Evans, G.Aromi, <i>CSD Communication(Private Communication)</i> (2004)

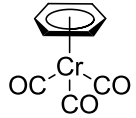
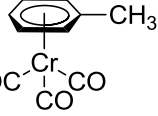
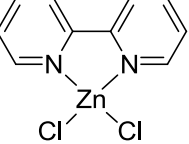
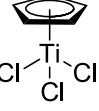
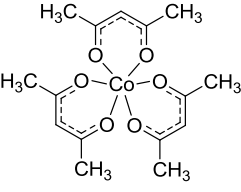
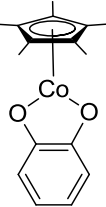
JAMMIT	(3,4-dihydroxyphenylacetyl)trimethylammonium chloride methanol solvate		R.B.Barlow, O.Johnson, J.A.K.Howard, D.C.Walton, G.Koellner, <i>Acta Crystallogr., Sect. B: Struct. Sci.</i> (1989), <b>45</b> , 396.
KOLDUL	(1R,2R)-1,2-diphenylethylenediammonium N-phenyliminodiacetate ethanol clathrate		Y.Imai, K.Murata, T.Sato, R.Kurodao, Y.Matsubara, <i>Org.Lett.</i> (2008), <b>10</b> , 3821.
MUTWUT	sodium 1-( $\alpha$ -L-threofuranosyl)thymine acetate		K.-U.Schoning, P.Scholz, Xiaolin Wu, S.Guntha, G.Delgado, R.Krishnamurthy, A.Eschenmoser, <i>Helv.Chim.Acta</i> (2002), <b>85</b> , 4111.
ROJJEG	N,N-dimethyl-3-phthalimidopropylammonium acetate hemihydrate		T.Borowiak, I.Wolska, P.Jensz, I.Kowalczyk, B.Brycki, A.Sztul, <i>J.Mol.Struct.</i> (2008), <b>891</b> , 205.
SIMRAI	isopropylammonium (isopropylamino)oxoacetate monohydrate		X.Sheng, C.E.Strasser, H.G.Raubenheimer, R.C.Luckay, <i>Acta Crystallogr., Sect. E: Struct. Rep. Online</i> (2007), <b>63</b> , o4361.

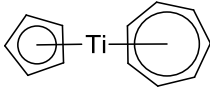
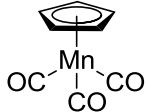
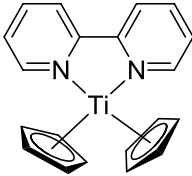
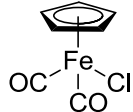
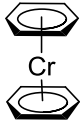
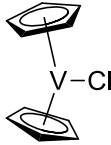
UGULUF	benzylammonium (4-chlorophenoxy)acetate monohydrate		Shouwen Jin, Zhanghui Lin, Daqi Wang, Guqing Chen, Zuoyi Ji, Tiansong Huang, Ying Zhou, <i>J.Chem.Cryst.</i> (2015), <b>45</b> , 159.
VEMJII	2-hydroxy-3-phenoxypropan-1-aminium hydroxy(phenyl)acetate monohydrate		Pei Wang, En Zhang, Jian-Feng Niu, Qing-Hua Ren, Peng Zhao, Hong-Min Liu, <i>Tetrahedron:Asymm.</i> (2012), <b>23</b> , 1046,
YEFVAH	(2S)-methyl 2-ammonio-3-(4-hydroxyphenyl)propionate chloride methanol solvate  (L-tyrosine methyl ester hydrochloride methanol solvate)		I.Bryndal, M.Jaremko, L.Jaremko, T.Lis, <i>Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.</i> (2006), <b>62</b> , o111

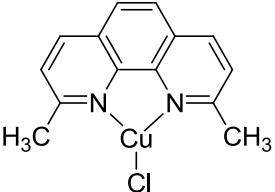
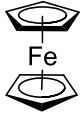
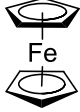
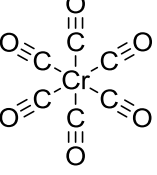
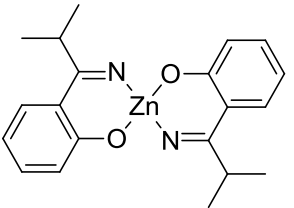
**Table S4** Crystal structure details for 63 metal organics, including solvates.

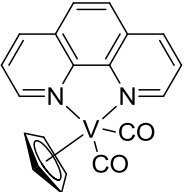
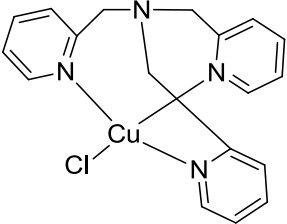
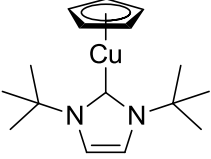
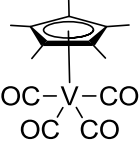
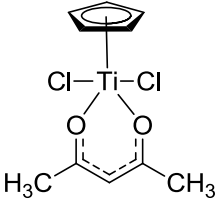
ACACCS	bis(2,4-pentanedionato) chromium(II)		F.A.Cotton, C.E.Rice, G.W.Rice, <i>Inorg.Chim.Acta</i> (1977), <b>24</b> , 231.
ACACMN0 2	tris(acetylacetonato)- manganese(iii)		J.P.Fackler Junior, A.Avdeef, <i>Inorg.Chem.</i> (1974), <b>13</b> , 1864
ACACSC	tris(acetylacetonato)- scandium(III)		T.J. Anderson, M.A. Neuman, G.A. Melson, <i>Inorg. Chem.</i> (1973), <b>12</b> , 927.
BENDAB	(4,4'-dimethyl-2,2'-bipyridine)- diacetato-zinc(II)		M.A.Harvey, S.A.Suarez, A.Ibanez, F.Doctorovich, R.Baggio, <i>Acta Crystallogr., Sect.E:Struct.Rep.Online</i> (2012), <b>68</b> , m1377.

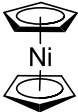
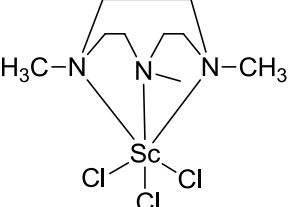
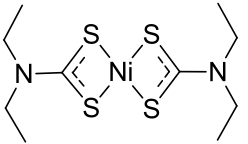
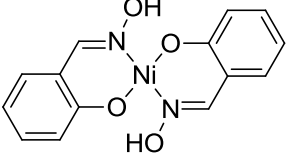
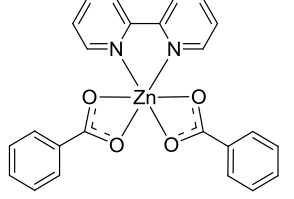


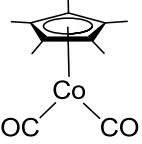
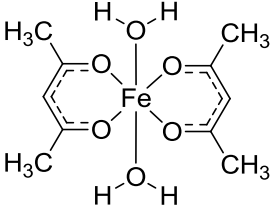
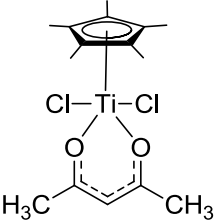
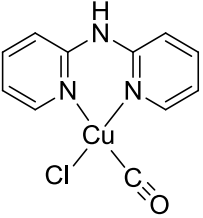
BZCRCO	( $\eta^6$ -benzene)-tricarbonyl-chromium(0)		M.F.Bailey, L.F.Dahl, <i>Inorg.Chem.</i> (1965), <b>4</b> , 1314.
CCRTOL	( $\eta^6$ -toluene)-tricarbonyl-chromium(0)		F.van Meurs, H.van Koningsveld, <i>J.Organomet.Chem.</i> (1977), <b>131</b> , 42.
CEFFOI	(2,2'-bipyridine)-dichloro-zinc(ii)		M.A.Khan, D.G.Tuck, <i>Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.</i> (1984), <b>40</b> , 60.
CEHPIO01	trichloro-( $\eta^5$ -cyclopentadienyl)-titanium(IV)		A.J.Rossini, R.W.Mills, G.A.Briscoe, E.L.Norton, S.J.Geier, I.Hung, Shaohui Zheng, J.Autschbach, R.W.Schurko, <i>J.Am.Chem.Soc.</i> (2009), <b>131</b> , 3317.
COACAC03	tris(acetylacetonato) cobalt(III)		G.J.Kruger, E.C.Reynhardt, <i>Acta Crystallogr.,Sect.B:Struct.Crystallogr.Cryst.Chem.</i> (1974), <b>30</b> , 822.
COSRUX	(o-catecholato-O,O')-( $\eta^5$ -pentamethyl-cyclopentadienyl)-cobalt(III)		E.J.Miller, A.L.Rheingold, T.B.Brill, <i>J.Organomet.Chem.</i> (1984), <b>273</b> , 377.

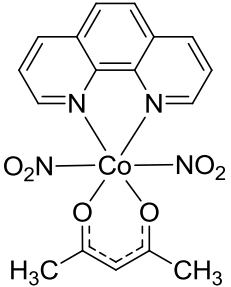
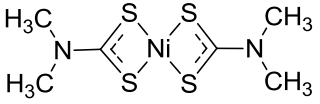
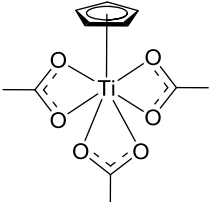
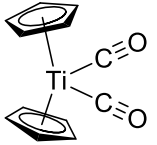
CPCHTI	( $\eta^5$ -cyclopentadienyl)-( $\eta^7$ -cycloheptatrienyl)-titanium		J.D.Zeinstra, J.L.de Boer, <i>J.Organomet.Chem.</i> (1973), <b>54</b> , 207.
CPMNCO01	tricarbonyl-( $\eta^5$ -cyclopentadienyl)-manganese(I)		P.J.Fitzpatrick, Y.Le Page, J.Sedman, I.S.Butler, <i>Inorg.Chem.</i> (1981), <b>20</b> , 2852.
CPTIBP01	(2,2'-bipyridyl)-bis( $\eta^5$ -cyclopentadienyl)-titanium		R.Gyepes, P.T.Witte, M.Horacek, I.Cisarova, K.Mach, <i>J.Organomet.Chem.</i> (1998), <b>551</b> , 207.
DADHIZ	dicarbonyl-chloro-( $\eta^5$ -cyclopentadienyl)-iron(II)		K.-J.Jens, E.Weiss, <i>Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.</i> (1985), <b>41</b> , 895.
DBENCR10	bis( $\eta^6$ -benzene)-chromium(0)		F.Jellinek, <i>J.Organomet.Chem.</i> (1963), <b>1</b> , 43.
DCPVCL	chloro-dicyclopentadienyl-vanadium		B.F.Fieselmann, G.D.Stucky, <i>J.Organomet.Chem.</i> (1977), <b>137</b> , 43.

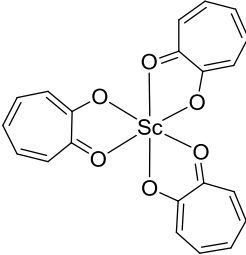
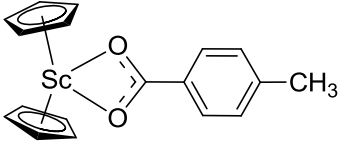
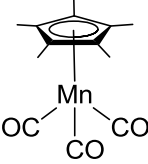
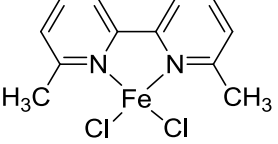
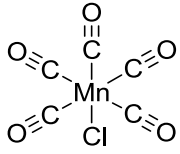
DIGWUL	chloro-(2,9-dimethyl-1,10-phenanthroline-N,N')-copper(I)		P.C.Healy, C.Pakawatchai, A.H.White, <i>J.Chem.Soc.,Dalton Trans.</i> (1985), 2531.
FEROCE06	ferrocene		F.Takusagawa, T.F.Koetzle, <i>Acta Crystallogr.,Sect.B:Struct.Crystallogr.Cryst.Chem.</i> (1979), <b>35</b> , 1074.
FEROCE27	ferrocene		C.P.Brock, Yigang Fu, <i>Acta Crystallogr.,Sect.B:Struct.Sci.</i> (1997), <b>53</b> , 928.
FOHCOU	hexacarbonyl-chromium(0)		A.Whitaker, J.W.Jeffery, <i>Acta Crystallogr.</i> (1967), <b>23</b> , 977.
FOMKIB01	bis(N-isopropylsalicylaldiminato-N,O)-zinc(II)		F.A.Bottino, P.Finocchiaro, E.Libertini, G.Mattern, <i>Z.Kristallogr.</i> (1989), <b>187</b> , 71.

FURRAL	dicarbonyl-( $\eta^5$ -cyclopentadienyl)- (2,2'-bipyridine-N,N')-vanadium		S.Gambarotta, A.Chiesi-Villa, C.Guastini, <i>Inorg.Chem.</i> (1988), <b>27</b> , 99.
GIHWIE01	chloro-(tris(2-pyridylmethyl)amine)-copper(I)		S.C.N.Hsu, S.S.C.Chien, H.H.Z.Chen, M.Y.Chiang, <i>J.Chin.Chem.Soc.(Taipei)</i> (2007), <b>54</b> , 685.
HEPSOL	(1,3-di-t-butyl-2,3-dihydroimidazol-2-ylidene)-( $\eta^5$ -cyclopentadienyl)-copper(I)		Hongping Ren, Xi Zhao, Shansheng Xu, Haibin Song, Baiquan Wang, <i>J.Organomet.Chem.</i> (2006), <b>691</b> , 4109.
JAFNAG	tetracarbonyl-( $\eta^5$ -pentamethyl-cyclopentadienyl)-vanadium		M.Herberhold, A.-M.Dietel, W.Milius, <i>Z.Naturforsch.,B:Chem.Sci.</i> (2003), <b>58</b> , 299.
JARNAS	(acetylacetonato)-dichloro-( $\eta^5$ -cyclopentadienyl)-titanium(IV)		Samkeun Lee, Kyoung-Chae Seo, Sock Sung Yun, Sung Kwon Kang, <i>J.Coord.Chem.</i> (2005), <b>58</b> , 695.

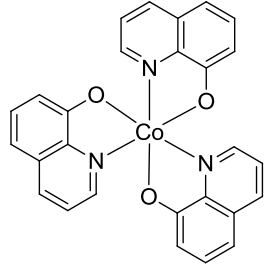
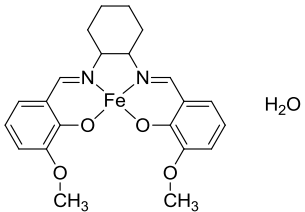
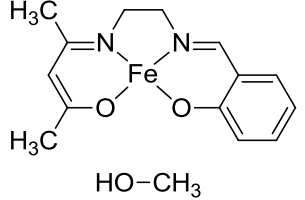
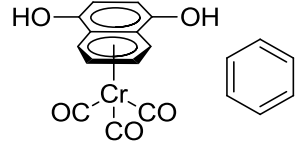
NCKLCN	nickelocene		P.Seiler, J.D.Dunitz, <i>Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem.</i> (1980), <b>36</b> , 2255.
NEZWEU	(1,4,7-trimethyl-1,4,7-triazacyclononane)-trichloroscandium		S.Hajela, W.P.Schaefer, J.E.Bercaw, <i>J.Organomet.Chem.</i> (1997), <b>532</b> , 45.
NIDCAR06	bis(N,N-diethyldithiocarbamato-S,S')-nickel(II)		A.Husain, S.A.A.Nami, S.P.Singh, M.Oves, K.S.Siddiqi, <i>Polyhedron</i> (2011), <b>30</b> , 33.
NISALO01	bis(salicylaldoximato-N,O)-nickel(II)		K.Mereiter, <i>CSD Communication (Private Communication)</i>
PESKEE01	bis(benzoato-O,O')-(2,2'-bipyridine-N,N')-zinc(ii)		Geun Hee Eom, Hyun Min Park, Min Young Hyun, Seung Pyo Jang, Cheal Kim, Jun Ho Lee, Suk Joong Lee, Sung-Jin Kim, Youngmee Kim, <i>Polyhedron</i> (2011), <b>30</b> , 1555.

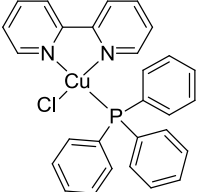
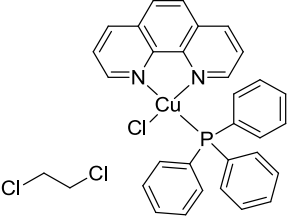
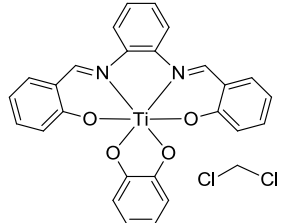
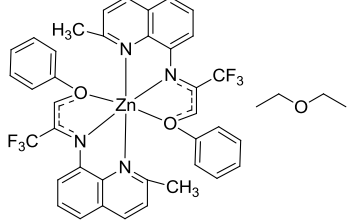
PMCCOC	dicarbonyl-(pentamethyl-cyclopentadienyl)-cobalt(I)		L.R.Byers, L.F.Dahl, <i>Inorg.Chem.</i> (1980), <b>19</b> , 277.
PVVBAY01	bis(acetylacetonato)-diaqua-Iron(II)		J.Laugier, J.P.Mathieu, <i>Acta Crystallogr.,Sect.B:Struct.Crystallogr.Cryst.Chem.</i> (1975), <b>31</b> , 631.
QENJAV	cis-dichloro-( $\eta^5$ -pentamethylcyclopentadienyl)-(2,4-pentanedionato)-titanium(IV)		Samkeun Lee, Sung Kwon Kang, Seung Jae Lee, Sock Sung Yun, Tae-Sun Chang, <i>Bull.Korean Chem.Soc.</i> (2005), <b>26</b> , 1620.
RUJBUT	carbonyl-chloro-(2,2'-dipyridylamine)-copper(I)		F.Ugozzoli, A.M.M.Lanfredi, N.Marsich, A.Camus, <i>Inorg.Chim.Acta</i> (1997), <b>256</b> , 1.

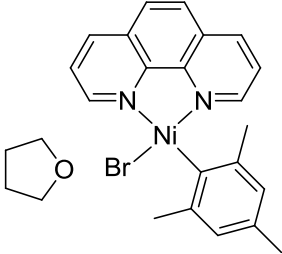
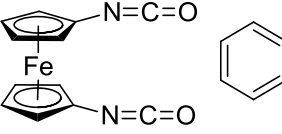
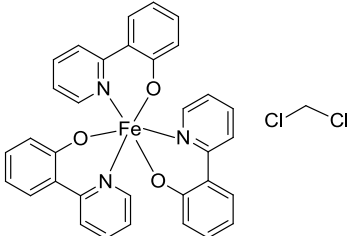
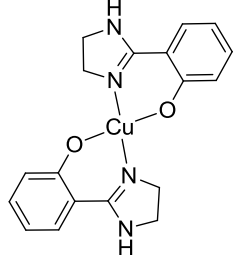
SAYVOE	bis(Nitrito-N)-(1,10-phenanthroline-N,N')-(2,4-pentanedionato-O,O')-cobalt(III)		Yun-Long Feng, Hong Lin, <i>Z.Kristallogr.-New Cryst.Struct.</i> (2005), <b>220</b> , 199.
TCBMNI	bis(N,N-dimethyldithiocarbamato)-nickel(II)		J.Lokaj, J.Garaj, V.Kettmann, V.Vrabel, <i>Collect.Czech.Chem.Comm.</i> (1980), <b>45</b> , 2147.
TESBUO	(η <sup>5</sup> -cyclopentadienyl)-tris(acetato-O,O')-titanium		Yujin Huang, N.Etkin, R.R.Heyn, T.T.Nadasdi, D.W.Stephan, <i>Organometallics</i> (1996), <b>15</b> , 2320.
TITODC10	dicarbonyl-dicyclopentadienyl-titanium(II)		J.L.Atwood, K.E.Stone, H.G.Alt, D.C.Hrncir, M.D.Rausch, <i>J.Organomet.Chem.</i> (1977), <b>132</b> , 367.

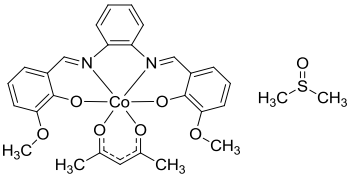
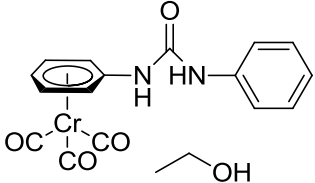
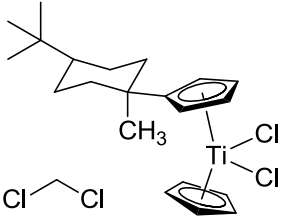
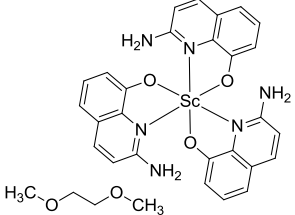
TROPSC	tris(tropolonato) scandium(III)		T.J.Anderson, M.A.Neuman, G.A.Melson, <i>Inorg.Chem.</i> (1974), <b>13</b> , 158.
VANPAB	bis( $\eta^5$ -pentamethyl-cyclopentadienyl)-(toluato-O,O')-scandium		M.A.St.Clair, B.D.Santarsiero, <i>Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.</i> (1989), <b>45</b> , 850
VIPGEG	tricarbonyl-( $\eta^5$ -pentamethyl-cyclopentadienyl)-manganese(I)		S.Fortier, M.C.Baird, K.F.Preston, J.R.Morton, T.Ziegler, T.J.Jaeger, W.C.Watkins, J.H.MacNeil, K.A.Watson, K.Hensel, Y.Le Page, J.-P.Charland, A.J.Williams, <i>J.Am.Chem.Soc.</i> (1991), <b>113</b> , 542
YABGAK	dichloro-(6,6'-dimethyl-2,2'-bipyridyl)-iron(II)		B.C.K.Chan, M.C.Baird, <i>Inorg.Chim.Acta</i> (2004), <b>357</b> , 2776,
ZOSWEJ	chloro-pentacarbonyl-manganese(I)		P.T.Greene, R.F.Bryan, <i>J.Chem.Soc.A</i> (1971), 1559,

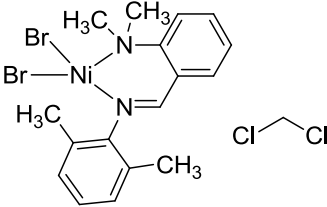
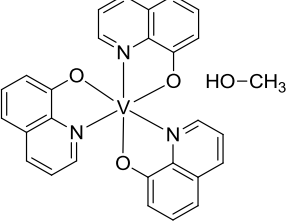


AJUJIY03	tris(8-quinolinolato-N,O)-cobalt(III) methanol solvate		D.Mandal, M.Mikuriya, Hoong-Kun Fun, D.Ray, <i>Inorg.Chem.Commun.</i> (2007), <b>10</b> , 657.
BOVNUW	(6,6'-dimethoxy-2,2'-diylbis(nitrilomethylidene)]diphenolato- $\kappa^4\text{O}^1, \text{N}, \text{N}', \text{O}^1$ )-iron(II) monohydrate		Peng-Fei Yan, Yan Bao, Hong-Feng Li, Guang-Ming Li, <i>Acta Crystallogr., Sect.E: Struct. Rep. Online</i> (2009), <b>65</b> , m832.
CAPVUM	(2-(((2-((4-(hydroxy)pent-3-en-2-ylidene)amino)ethyl)imino)methyl)phenolato)-nickel methanol solvate		Jia-Zhong Wang, Jing-Chi Gu, Xue-Cheng Zhang, Jing Huang, Bi-Xue Zhu, <i>Wuji Huaxue Xuebao (Chin.) (Chin. J. Inorg. Chem.)</i> (2012), <b>28</b> , 321.
CECGIB	$(\eta^6\text{-}1,4\text{-dihydroxynaphthalene})\text{-tricarbonyl-chromium benzene solvate}$		E.P.Kundig, A.E.Garcia, T.Lomberget, G.Bernardinelli, <i>Angew.Chem., Int.Ed.</i> (2006), <b>45</b> , 98.

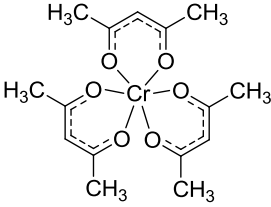
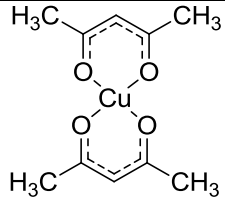
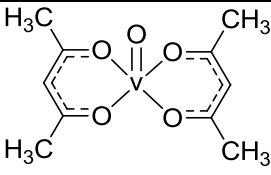
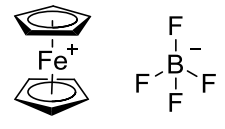
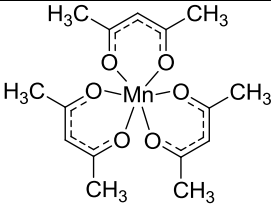
CEKHOP	2,2'-bipyridine-chloro-triphenylphosphine-copper(i) monohydrate		B.E.Green, C.H.L.Kennard, G.Smith, B.D.James, A.H.White, <i>Acta Crystallogr., Sect. C: Cryst. Struct. Commun.</i> (1984), <b>40</b> , 426.
COXSOZ	chloro-(1,10-phenanthroline)-(triphenylphosphine)-copper 1,2-dichloroethane solvate		L.I.Panferova, F.M.Miloserdov, Anton Lishchynskyi, M.M.Belmonte, J.Benet-Buchholz, V.V.Grushin, <i>Angew.Chem., Int.Ed.</i> (2015), <b>54</b> , 5218.
DARCIK	(benzene-1,2-diolato)-(2,2'-(1,2-phenylenebis((nitrido)methylidene))bis(4-methylphenolato))-titanium dichloromethane solvate		A.Tzubery, E.Y.Tshuva, <i>Inorg.Chem.</i> (2012), <b>51</b> , 1796.
DOQGOH	bis(4,4,4-trifluoro-3-((2-methylquinolin-8-yl)amino)-1-phenylbut-2-en-1-onato)-zinc diethyl ether solvate		K.A.Gerling, N.M.Rezayee, A.L.Rheingold, D.B.Green, J.M.Fritsch, <i>Dalton Trans.</i> (2014), <b>43</b> , 16498.

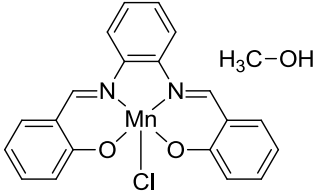
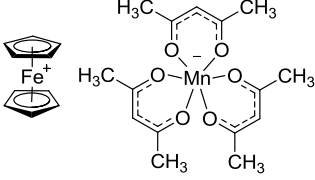
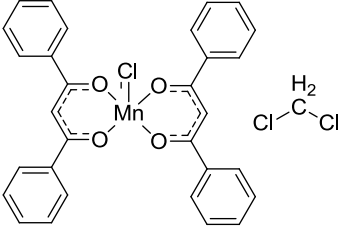
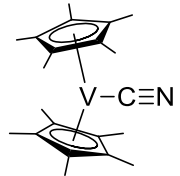
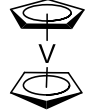
FIQXAG	bromo-mesityl-(1,10-phenanthroline)-nickel tetrahydrofuran solvate		D.G.Yakhvarov, A.Petr, V.Kataev, B.Buchner, S.Gomez-Ruiz, E.Hey-Hawkins, S.V.Kvashennikova, Y.S.Ganushevich, V.I.Morozov, O.G.Sinyashin, <i>J.Organomet.Chem.</i> (2014), <b>750</b> , 59.
FIXJON	1,1'-diisocyanatoferrrocene benzene solvate		A.R.Petrov, K.Jess, M.Freytag, P.G.Jones, M.Tamm, <i>Organometallics</i> (2013), <b>32</b> , 5946.
GAPMIT	tris(2-(o-hydroxyphenyl)-pyridine-O,N)-cobalt(III) dichloromethane solvate		P.Ganis, A.Saporito, A.Vitagliano, G.Valle, <i>Inorg.Chim.Acta</i> (1988), <b>142</b> , 75.
JEVMIH	bis(2-(4,5-dihydro-1H-imidazol-2-yl)phenolato-N,O)-zinc(ii) methanol solvate		Hong-Shan He, <i>Acta Crystallogr.,Sect.E:Struct.Rep.Online</i> (2007), <b>63</b> , m344.

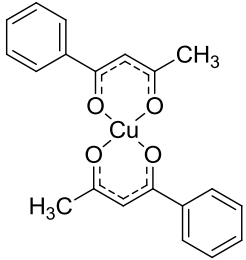
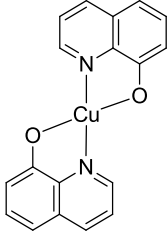
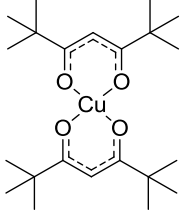
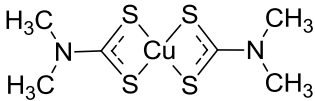
KUHRIQ	(acetylacetonato)-(2,2'-(ethane-1,2-diylbis(nitrilomethylidene))bis(6-methoxyphenolato))-cobalt(III) dimethyl sulfoxide solvate		C.Schieber, J.Howitt, U.Putz, J.M.White, C.L.Parish, P.S.Donnely, Seong-Seng Tan, <i>J.Biol.Chem.</i> (2011), <b>286</b> , 8555.
MAHWAV	tricarbonyl-( $\eta^6$ -1,3-diphenylurea)-chromium ethanol solvate		Xiaohui Tian, Li Song, Yizhong Yuan, Jiaping Lin, <i>Organometallics</i> (2010), <b>29</b> , 509.
MOLPOT	( $\eta^5$ -(4-t-butyl-1-methyl-1-cyclohexyl)cyclopentadienyl)-dichloro-( $\eta^5$ -cyclopentadienyl)-titanium(IV) dichloromethane solvate		A.Gansauer, I.Winkler, D.Worgull, D.Franke, T.Lauterbach, A.Okkel, M.Nieger, <i>Organometallics</i> (2008), <b>27</b> , 5699.
OVIMAI	tris(2-aminoquinolin-8-olato)-scandium 1,2-dimethoxyethane solvate		M.A.Katkova, T.V.Balashova, A.P.Pushkarev, I.Yu.Ilyin, G.K.Fukin, E.V.Baranov, S.Yu.Ketkov, M.N.Bochkarev, <i>Dalton Trans.</i> (2011), <b>40</b> , 771.

PEKNOK	(2-(((2,6-dimethylphenyl)imino)methyl)-N,N-dimethylaniline)-dibromonickel dichloromethane solvate		Jun-Kai Zhang, Peng-Chao Wang, Xiao-Wei Wang, Liang Wang, Jun-Cai Chen, Zhi-Wu Zheng, Yong-Ping Niu, <i>J.Organomet.Chem.</i> (2011), <b>696</b> , 3697.
QOFHOI	tris(8-oxyquinoline)-vanadium(III) methanol solvate		M.J.Manos, A.J.Tasiopoulos, C.Raptopoulou, A.Terzis, J.D.Woollins, A.M.Z.Slawin, A.D.Keramidas, T.A.Kabanos, <i>J.Chem.Soc.,Dalton Trans.</i> (2001), 1556.

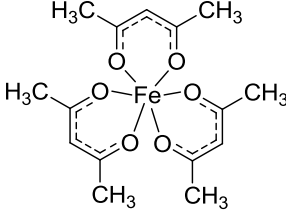
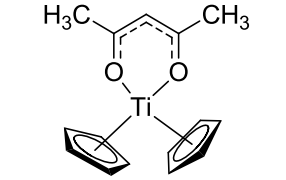
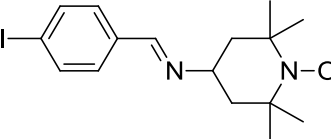
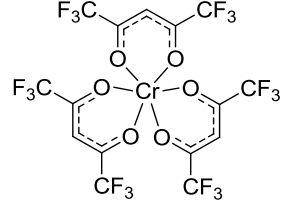
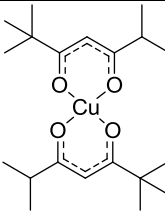
**Table S5** Crystal structure details for 27 open shell pairs.

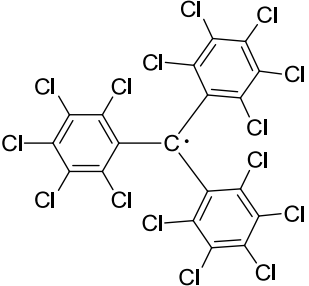
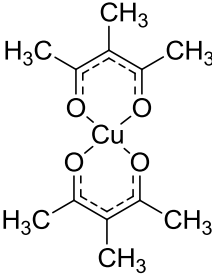
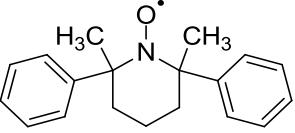
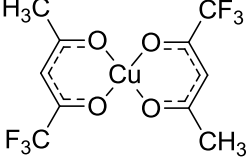
ACACCR07	tris(acetylacetonato)-chromium(III)		L.S.von Chrzanowski, M.Lutz, A.L.Spek, <i>Acta Crystallogr., Sect. C: Cryst. Struct. Commun.</i> (2007), <b>63</b> , m377.
ACACCU02	bis(acetylacetonato)-copper(II)		G.Berry, G.Callon, B.Gowans, J.N.Low, R.Smith, <i>CSD Communication(Private Communication)</i> (2004)
ACACVO04	bis(acetylacetonato)-oxo-vanadium(IV)		M.Hoshino, A.Sekine, H.Uekusa, Y.Ohashi, <i>Chem.Lett.</i> (2005), <b>34</b> , 1228.
AFALID01	ferrocenium tetrafluoroborate		S.R.Posner, L.C.Lorson, A.R.Gell, B.M.Foxman, <i>Cryst.Growth Des.</i> (2015), <b>15</b> , 3407.
ACACMN2 1	tris(acetylacetonato)-manganese(III)		B.R.Stults, R.S.Marianelli, V.W.Day, <i>Inorg.Chem.</i> (1979), <b>18</b> , 1853.

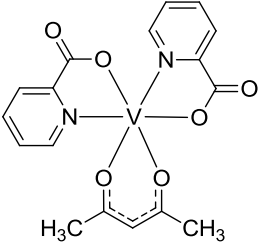
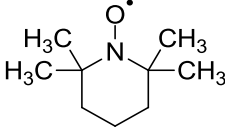
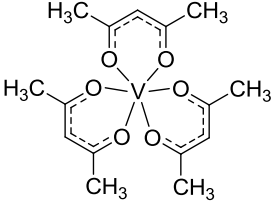
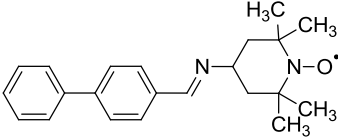
AFATAE	chloro-(2,2'-(1,2-phenylenebis((nitrilo)methylidene))diphenolato)-manganese(III) methanol solvate		H.Lin, J.-G.Wang, H.-T.Shi, Q.Chen, Q.-F.Zhang, <i>Acta Crystallogr., Sect. E: Struct. Rep. Online</i> (2013), <b>69</b> , m404.
AGEFEX	ferrocenium tris(hexafluoroacetylacetonato)-manganese(II)		J.R.Bryant, J.E.Taves, J.M.Mayer, <i>Inorg. Chem.</i> (2002), <b>41</b> , 2769.
BEPRET	bis(dibenzoylmethane)-chloro-manganese(III) dichloromethane solvate		G.Aromi, M.J.Knapp, J.-P.Claude, J.C.Huffman, D.N.Hendrickson, G.Christou, <i>J. Am. Chem. Soc.</i> (1999), <b>121</b> , 5489.
CIRSEB	cyano-bis(η <sup>5</sup> -pentamethyl-cyclopentadienyl)-vanadium		S.Gambarotta, C.Floriani, A.Chiesi-Villa, C.Guastini, <i>Inorg. Chem.</i> (1984), <b>23</b> , 1739.
CPNDYV07	bis(η <sup>5</sup> -cyclopentadienyl)-vanadium		A.L.Spek, <i>CSD Communication (Private Communication)</i> (2000)

CUBEAC01	bis(benzoylacetato)-copper(II)		S.K.Dey, B.Bag, Zhongyuan Zhou, A.S.C.Chan, S.Mitra, <i>Inorg.Chim.Acta</i> (2004), <b>357</b> , 1991.
CUQUIN05	bis(8-hydroxyquinolino-N,O)-copper(II)		S.Ammor, G.Coquerel, G.Perez, F.Robert, <i>Eur.J.Solid State Inorg.Chem.</i> (1992), <b>29</b> , 445.
DERNOD05	bis(2,2,6,6-tetramethyl-3,5-heptanedionato)-copper(II)		M.Hamid, M.Mazhar, M.Zeller, A.D.Hunter, <i>CSD Communication(Private Communication)</i> (2005)
DMTCCU	bis(N,N-dimethyldithiocarbamate)-copper(II)		F.W.B.Einstein, J.S.Field, <i>Acta Crystallogr.,Sect.B:Struct.Crystallogr.Cryst.Chem.</i> (1974), <b>30</b> , 2928.



FEACAC03	tris(acetylacetonato)-iron(III)		M.-L.Hu, Z.-M.Jin, Q.Miao, L.-P.Fang, <i>Z.Kristallogr.-New Cryst.Struct.</i> (2001), <b>216</b> , 597.
HIDPOZ	(acetylacetonato-O,O')-titanocene(III)		A.M.Bond, R.Colton, U.Englert, H.Hugel, F.Marten, <i>Inorg.Chim.Acta</i> (1995), <b>235</b> , 117.
HIRNEB	4-(4-fluorophenyl)-methyleneamino-2,2,6,6-tetramethylpiperidin-1-oxyl radical		F.Iwasaki, J.H.Yoshikawa, H.Yamamoto, E.Kan-nari, K.Takada, M.Yasui, T.Ishida, T.Nogami, <i>Acta Crystallogr.,Sect.B:Struct.Sci.</i> (1999), <b>55</b> , 231.
IGAGEC	tris(1,1,1,5,5,5-hexafluoroacetylacetonato)-chromium(III)		P.G.Jessop, M.M.Olmstead, C.D.Ablan, M.Grabenauer, D.Sheppard, C.A.Eckert, C.L.Liotta, <i>Inorg.Chem.</i> (2002), <b>41</b> , 3463.
IPEZOS	bis(2,2,6-trimethylheptane-3,5-dionato)-copper(II)		M.J.Delarosa, K.S.Bousman, J.T.Welch, P.J.Toscano, <i>J.Coord.Chem.</i> (2003), <b>56</b> , 1339.

JIYKEH01	perchlorotriptyl radical		J.Guasch, X.Fontrodona, I.Ratera, C.Rovira, J.Veciana, <i>Acta Crystallogr., Sect.C:Cryst.Struct.Commun.</i> (2013), <b>69</b> , 255.
MACACU1 0	bis(3-methylpentane-2,4-dionato)- copper(II)		I.Robertson, M.R.Truter, <i>J.Chem.Soc.A</i> (1967), 309.
POXYUW	rac-trans-2,6-dimethyl-2,6- diphenylpiperidine N-oxide		J.Einhorn, C.Einhorn, F.Ratajczak, A.Durif, M.-T.Averbuch, J.-L.Pierre, <i>Tetrahedron Lett.</i> (1998), <b>39</b> , 2565.
QQQBWP0 3	trans-bis(1,1,1-trifluoropentan- 2,4-dionato)-copper(ii)		R.E.Marsh, <i>Acta Crystallogr.,Sect.B:Struct.Sci.</i> (2009), <b>65</b> , 782.

SUZSAH	(acetylacetonato-O,O')-bis(picolinato-N,O)-manganese(III)		T.Nakamura, K.Niwa, S.Usugi, H.Asada, M.Fujiwara, T.Matsushita, <i>Polyhedron</i> (2001), <b>20</b> , 191
TMPPIO13	2,2,6,6-tetramethylpiperidine-1-oxyl		S.Spirk, F.Belaj, T.Madl, R.Pietschnig, <i>Eur.J.Inorg.Chem.</i> (2010), 289.
VAACAC02	tris(2,4-pentanedionato-O,O')-vanadium(III)		C.A.L.Filgueiras, A.Horn Junior, R.A.Howie, J.M.S.Skakle, J.L.Wardell, <i>Acta Crystallogr.,Sect.E:Struct.Rep.Online</i> (2001), <b>57</b> , m157
YUJYIL01	4-((4-phenylbenzylidene)amino)-2,2,6,6-tetramethylpiperidine-1-oxyl radical		F.Iwasaki, J.H.Yoshikawa, H.Yamamoto, E.Kan-nari, K.Takada, M.Yasui, T.Ishida, T.Nogami, <i>Acta Crystallogr.,Sect.B:Struct.Sci.</i> (1999), <b>55</b> , 231